A.1

DERIVATION OF THE X-RAY FORM FACTOR

An X-ray beam is incident in the direction defined by the unit vector s_0. We shall consider radiation scattered in the direction defined by the unit vector s [7]

The path difference between the rays is:

$$OR - QP = r.S - r.S_0 \qquad \text{… (A.1-1)}$$

Phase difference $= \frac{2\pi}{\lambda} \times$ path difference

Where λ is the wavelength of the incident radiation

Then

$$\text{Phase difference} = \frac{2\pi}{\lambda} \vec{r}.(\vec{s} - \vec{s}_0) \qquad \text{… (A.1-2)}$$

Hence the scattered amplitude from an element dr of electron density $\rho(r)$ is given by:

$$\text{Scattered amplitude} = \rho(r) e^{\frac{2\pi i}{\lambda} \vec{r}.(\vec{s} - \vec{s}_0)} dr \qquad \text{… (A.1-3)}$$

$$= \rho(r) e^{ik\vec{d}.\vec{r}} dr \qquad \text{… (A.1-4)}$$

Where $k = \frac{2\pi}{\lambda}$, $\vec{d} = \vec{s} - \vec{s}_0$

Thus, the total scattered amplitude is obtained by integration over the whole electron density distribution as:

$$\text{Total scattered amplitude} \propto \int \rho(r) e^{ik\vec{d}.\vec{r}} dr \qquad \text{… (A.1-5)}$$

Let us write the atomic scattering factor $f(s)$ from an electron distribution of density $\rho(r)$ as $s = kd$

For closed shell atom $\rho(r)$ is spherically symmetrical.

The angular integrations can then be performed by spherical polar coordinates r, θ, ϕ.

Then the volume element becomes $r^2 dr \sin\theta d\theta d\phi$, and since $s.r = sr\cos\theta$ we can integrate over ϕ from 0 to 2π to obtain.

$$f(s) = 2\pi \int_0^\infty r^2 \rho(r) dr \int_0^\pi e^{isr\cos\theta} \sin\theta d\theta \qquad \text{… (A.1-6)}$$

The integration over θ can be carried out, with the result

$$f(s) = \int_0^\infty \frac{\sin sr}{sr} \rho(r) 4\pi r^2 dr \qquad \text{… (A.1-7)}$$

But $\rho(r) 4\pi r^2 = D(r)$ … (A.1-8)

Then

$$f(s) = \int_0^\infty D(r) \frac{\sin sr}{sr} dr \qquad \text{… (A.1-9)}$$

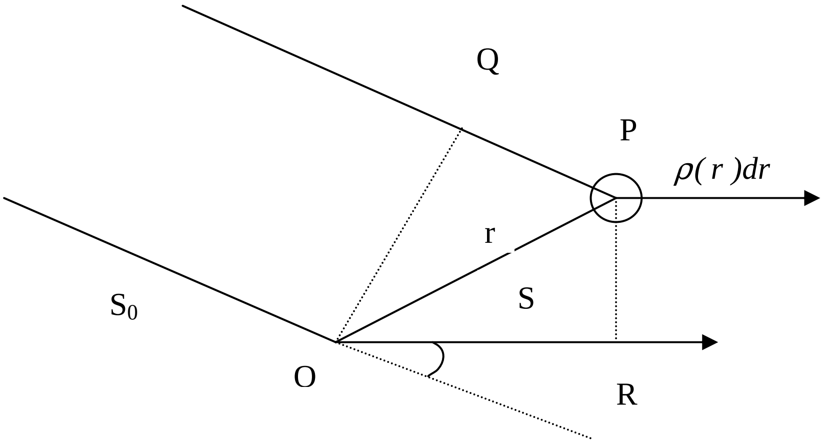

Fig.(A.1-1) x-ray scattering

The solution of equation (A.1-9) by mathematical analysis is:

For K-shell

$$D(r) = \sum_i \sum_j N_i N_j e^{-(\zeta_i+\zeta_j).r} r^{(n_i+n_j)} \qquad \text{… (A.1-10)}$$

$$\sin(sr) = sr - \frac{(sr)^3}{3!} + \frac{(sr)^5}{5!} - ...... \qquad \text{… (A.1-11)}$$

By substituting equation (A.1-11) and (A.1-10) in equation (A.1-9)

$$f(s) = \int_0^\infty \left[\sum_i \sum_j c_i c_j N_i N_j e^{-(\zeta_i+\zeta_j).r} r^{(n_i+n_j)} \right] \left[\frac{sr - \frac{(sr)^3}{3!} + \frac{(sr)^5}{5!} - ......}{sr} \right] dr$$

… (A.1-12)

$$x = \sum_i \sum_j c_i c_j N_i N_j \qquad \text{… (A.1-13)}$$

$$m = \zeta_i + \zeta_j \qquad \text{… (A.1-14)}$$

$$p = n_i + n_j \qquad \text{… (A.1-15)}$$

$$f(s) = x\int_0^\infty r^p e^{-m.r} (1 - \frac{(sr)^2}{3!} + \frac{(sr)^4}{5!} - ......) dr$$

$$= x\int_0^\infty \left[r^p e^{-m.r} - \frac{s^2}{3!} r^{p+2} e^{-m.r} + \frac{s^4}{5!} r^{p+4} e^{-m.r} \right] dr$$

$$= x\left[\frac{p!}{m^{p+1}} - \frac{s^2}{3!} \frac{(p+2)!}{m^{p+3}} + \frac{s^4}{5!} \frac{(p+4)!}{m^{p+5}} \right]$$

$$f(s) = x\left[\sum_{k=0}(-1)^k \frac{(p+2(k))!\, s^{2(k)}}{(2(k)+1)!\, m^{p+2(k)+1}}\right] \qquad \text{… (A.1-16)}$$

$$f(s) \ = \sum_i \sum_j c_i c_j N_i N_j \left[\sum_{k=0}(-1)^k \frac{\left(n_i + n_j + 2(k)\right)!\, s^{2(k)}}{(2(k)+1)!\left(\zeta_i + \zeta_j\right)^{n_i+n_j+2(k)+1}}\right] \qquad \text{… (A.1-17)}$$

The total scattering form factor is given by:

For Li-like ions

$$f(s)_{total} = 3\left[\int_0^\infty D_T(r_1)\frac{sin(sr_1)}{sr_1}dr_1\right] \qquad \text{… (A.1-18)}$$

$$D_T(r_1) = \frac{1}{3}\left[D_{K\alpha K\beta}(r_1) + D_{K\alpha L\alpha}(r_1) + D_{K\beta L\alpha}(r_1)\right]$$

$$f(s) = 2\sum_i \sum_j c_i c_j N_i N_j \left[\sum_{p=0}(-1)^p \frac{\left(n_i + n_j + 2(p)\right)!\, s^{2(p)}}{(2(k)+1)!\left(\zeta_i + \zeta_j\right)^{n_i+n_j+2(p)+1}}\right] + \sum_i \sum_j d_i d_j N_i N_j \left[\sum_{p=0}(-1)^p \frac{\left(n_i + n_j + 2(p)\right)!\, s^{2(p)}}{(2(k)+1)!\left(\zeta_i + \zeta_j\right)^{n_i+n_j+2(p)+1}}\right]\Bigg) \qquad \text{… (A.1-19)}$$

For Be-like ions

$$f(s)_{total} = 4\left[\int_0^\infty D_T(r_1)\frac{sin(sr_1)}{sr_1}dr_1\right] \qquad \text{… (A.1-20)}$$

$$D_T(r_1)=\frac{1}{6}\left[D_{K\alpha K\beta}(r_1)+D_{K\alpha L\alpha}(r_1)+D_{K\beta L\alpha}(r_1)+D_{K\alpha L\beta}(r_1)+D_{K\beta L\beta}(r_1)+D_{L\alpha L\beta}(r_1)\right]$$

$$\begin{aligned}f(s)=3\sum_i\sum_j c_i c_j N_i N_j&\left[\sum_{p=0}(-1)^p\frac{\left(n_i+n_j+2(p)\right)!\,s^{2(p)}}{(2(k)+1)!\left(\zeta_i+\zeta_j\right)^{n_i+n_j+2(p)+1}}\right]\\+3\sum_i\sum_j d_i d_j N_i N_j&\left[\sum_{p=0}(-1)^p\frac{\left(n_i+n_j+2(p)\right)!\,s^{2(p)}}{(2(k)+1)!\left(\zeta_i+\zeta_j\right)^{n_i+n_j+2(p)+1}}\right]\end{aligned}$$

… (A.1-21)

A.2

DERIVATIONS THE TWO-PARTICLE DENSITY $\Gamma_{HF}(1,2)$ FOR $K_\alpha K_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ and, $L_\alpha L_\beta$

The two-particle density function $\Gamma_{HF}(1,2)$ for the individual shells for Li-Like ions can be written as [51]:

$$\Gamma_{ij}(1,2)=\frac{1}{2}\sum_{i<j}^{3}A_{ij}^{*}A_{ij}$$

And for Be-like ions can be written as:

$$\Gamma_{ij}(1,2)=\frac{1}{2}\sum_{i<j}^{6}A_{ij}^{*}A_{ij}$$

i	j	$\Gamma_{ij}(1,2)$	Shell
1	2	$\Gamma_{12}(1,2)$	$K_\alpha K_\beta$
1	3	$\Gamma_{13}(1,2)$	$K_\alpha L_\alpha$
2	3	$\Gamma_{23}(1,2)$	$K_\beta L_\alpha$
1	4	$\Gamma_{14}(1,2)$	$K_\alpha L_\beta$
2	4	$\Gamma_{24}(1,2)$	$K_\beta L_\beta$
3	4	$\Gamma_{34}(1,2)$	$L_\alpha L_\beta$

$$A_{ij}=\phi_i(1)\phi_j(2)-\phi_j(1)\phi_i(2) \qquad \text{… (A.2.1)}$$

In this work $A_{ij}^{\bullet}\equiv A_{ij}$ due to the S-state symmetry.

(1) $K_\alpha K_\beta$ Shell:

$$\Gamma_{12}(1,2)=\frac{1}{2}\left[\phi_1(1)\phi_2(2)-\phi_2(1)\phi_1(2)\right]^2$$ …(A.2.2)

$$\Gamma_{12}=\frac{1}{2}[\varphi_{1s}(1)\alpha(1)\varphi_{1s}(2)\beta(2)-\phi_{1s}(1)\beta(1)\phi_{1s}(2)\alpha(2)$$ …(A.2.4)

Since :

$$\left.\begin{aligned}\varphi_{1s}(1)&=R_{1s}(1)Y_{1s}(1)\\ \varphi_{1s}(2)&=R_{1s}(2)Y_{1s}(2)\end{aligned}\right\}$$ …(A.2.5)

After integrated over all spins in equation (A.2.4) and substituted equation (A.2.5) into (A.2.4) we get:

$$\Gamma'_{12}(spinless)=\left[R_{1s}(1)Y_{1s}(1)R_{1s}(2)Y_{1s}(2)\right]^2$$ ….(A.2.6)

now we can integrate over all angular part to get:

$$\Gamma'_{12}(1,2)=R_{1s}{}^2(1)R_{1s}{}^2(2)$$ …(A.2.7)

(2) $K_\alpha L_\alpha$ Shell:

$$\Gamma_{13}(1,2)=\frac{1}{2}\left[\phi_1(1)\phi_3(2)-\phi_3(1)\phi_1(2)\right]^2$$ …(A.2.8)

$$\Gamma_{13}(1,2)=\frac{1}{2}\left[\varphi_{1s}(1)\alpha(1)\varphi_{2s}(2)\alpha(2)-\varphi_{2s}(1)\alpha(1)\varphi_{1s}(2)\alpha(2)\right]^2$$ ...(A.2.9)

$$\Gamma_{13}(1,2)=[\alpha(1)\alpha(2)]^2\left[\frac{\varphi_{1s}(1)\varphi_{2s}(2)-\varphi_{2s}(1)\varphi_{1s}(2)}{\sqrt{2}}\right]^2 \qquad \text{…(A.2.10)}$$

since

$$\left.\begin{aligned}\varphi_{1s}(1)&=R_{1s}(1)Y_{1s}(1)\\ \varphi_{1s}(2)&=R_{1s}(2)Y_{1s}(2)\\ \varphi_{2s}(1)&=R_{2s}(1)Y_{2s}(1)\\ \varphi_{2s}(2)&=R_{2s}(2)Y_{2s}(2)\end{aligned}\right\} \qquad \text{…(A.2.11)}$$

And

$$\left.\begin{aligned}\int\alpha(1)\beta(1)d\sigma&=0\\ \int\alpha(1)\alpha(1)d\sigma&=1\\ \int\beta(1)\alpha(1)d\sigma&=0\\ \int\beta(1)\beta(1)d\sigma&=1\end{aligned}\right\} \qquad \text{…(A.2.12)}$$

by substituted the equation (A.2.11) into (A.2.10) and integrated over all spins using equation (A.2.12) we get:

$$\Gamma'_{13}(spinless)=\frac{1}{2}[R_{1s}(1)Y_{1s}(1)R_{2s}(2)Y_{2s}(2)-R_{2s}(1)Y_{2s}(1)R_{1s}(2)Y_{1s}(2)]^2 \qquad \text{….(A.2.13)}$$

Since

$$Y_{1s}(\theta,\varphi)=Y_{2s}(\theta,\varphi) \qquad \text{…(A.2.14)}$$

$$\Gamma'_{13}(1,2)=\frac{1}{2}[Y_{1s}(1)Y_{2s}(2)]^2[R_{1s}(1)R_{2s}(2)-R_{2s}(1)R_{1s}(2)]^2 \qquad \text{…(A.2.15)}$$

Now we can integrate over all the angular part so that we can get:

$$\Gamma_{13}(1,2)=\left[\frac{R_{1s}(1)R_{2s}(2)-R_{2s}(1)R_{1s}(2)}{\sqrt{2}}\right]^2 \qquad \text{…(A.2.16)}$$

$$\Gamma_{13}{}'(1,2)=\frac{1}{2}\left[R_{1s}^2(1)R_{2s}^2(2)+R_{2s}^2(1)R_{1s}^2(2)\right.$$
$$\left.-2R_{1s}(1)R_{2s}(1)R_{2s}(2)R_{1s}(2)\right]$$
….(A.2.17)

(3) $K_\beta L_\alpha$ **Shell:**

$$\Gamma_{23}(1,2)=\frac{1}{2}\left[\phi_2(1)\phi_3(2)-\phi_3(1)\phi_2(2)\right]^2 \qquad \text{…(A.2.18)}$$

$$\Gamma_{23}(1,2)=\frac{1}{2}\left[\varphi_{1s}(1)\beta(1)\varphi_{2s}(2)\alpha(2)-\varphi_{2s}(1)\alpha(1)\varphi_{1s}(2)\beta(2)\right]^2$$
..(A.2.19)

By substituted equation (A.2.11) into (A.2.19) and integrated over all spins using equation (A.2.12) we get:

$$\Gamma'_{23}(spinless)=\frac{1}{2}\left[R_{1s}^2(1)Y_{1s}^2(1)R_{2s}^2(2)Y_{2s}^2(2)+R_{2s}^2(1)Y_{2s}^2(1)R_{1s}^2(2)Y_{1s}^2(2)\right]$$
…(A.2.20)

Using eq.(A.2.14) and integrate over all angular part to get:

$$\Gamma'_{23}(1,2)=\frac{1}{2}\left[R_{1s}^2(1)R_{2s}^2(2)+R_{2s}^2(1)R_{1s}^2(2)\right] \qquad \text{…(A.2.21)}$$

(4) $K_\alpha L_\beta$ **shell**

$$\Gamma_{14}(1,2)=\frac{1}{2}\left[\phi_1(1)\phi_4(2)-\phi_4(1)\phi_1(2)\right]^2$$ ...(A.2.22)

$$\Gamma_{14}(1,2)=\frac{1}{2}\left[\varphi_{1s}(1)\alpha(1)\varphi_{2s}(2)\beta(2)-\varphi_{2s}(1)\beta(1)\varphi_{1s}(2)\alpha(2)\right]^2$$

..(A.2.23)

By substituting equation (A.2.11) into (A.2.23) and integrated over all spins using equation (A.2.12) we get:

$$\Gamma'_{14}(spinless)=\frac{1}{2}\left[R_{1s}^2(1)Y_{1s}^2(1)R_{2s}^2(2)Y_{2s}^2(2)+R_{2s}^2(1)Y_{2s}^2(1)R_{1s}^2(2)Y_{1s}^2(2)\right]$$

...(A.2.24)

using equation (A.2.14) and integrate over all angular part to get:

$$\Gamma'_{14}(1,2)=\frac{1}{2}\left[R_{1s}^2(1)R_{2s}^2(2)+R_{2s}^2(1)R_{1s}^2(2)\right]$$ ...(A.2.25)

(5)* $K_\beta L_\beta$ Shell*:

$$\Gamma_{24}(1,2)=\frac{1}{2}\left[\phi_2(1)\phi_4(2)-\phi_4(1)\phi_2(2)\right]^2$$ ...(A.2.26)

$$\Gamma_{24}(1,2)=\frac{1}{2}\left[\varphi_{1s}(1)\beta(1)\varphi_{2s}(2)\beta(2)-\varphi_{2s}(1)\beta(1)\varphi_{1s}(2)\beta(2)\right]^2$$

...(A.2.27)

By substituting equation (A.2.11) into (A.2.27) and integrated over all spins using equation (A.2.12) we get:

$$\Gamma'_{24}(\,spinless\,)=\frac{1}{2}\left[R_{1s}^{2}(1)Y_{1s}^{2}(1)R_{2s}^{2}(\,2\,)Y_{2s}^{2}(\,2\,)+R_{2s}^{2}(1)Y_{2s}^{2}(1)R_{1s}^{2}(\,2\,)Y_{1s}^{2}(\,2\,)\right]$$

...(A.2.28)

using equation (A.2.14) and integrate over all angular part to get:

$$\begin{aligned}\Gamma_{24}{}'(1{,}2\,)=\frac{1}{2}\big[&R_{1s}^{2}(1)R_{2s}^{2}(\,2\,)+R_{2s}^{2}(1)R_{1s}^{2}(\,2\,)\\&-2R_{1s}(1)R_{2s}(1)R_{2s}(\,2\,)R_{1s}(\,2\,)\big]\end{aligned}$$

...(A.2.29)

(6) $L_{\alpha}L_{\beta}$ **shell**:

$$\Gamma_{34}(1{,}2\,)=\frac{1}{2}\left[\phi_{3}(1)\phi_{4}(\,2\,)-\phi_{4}(1)\phi_{3}(\,2\,)\right]^{2}$$

...(A.2.30)

$$\Gamma_{34}(1{,}2\,)=\frac{1}{2}\left[\varphi_{2s}(1)\alpha(1)\varphi_{2s}(\,2\,)\beta(\,2\,)-\phi_{2s}(1)\beta(1)\phi_{2s}(\,2\,)\alpha(\,2\,)\right]^{2}$$

...(A.2.31)

Since :

$$\left.\begin{aligned}\varphi_{2s}(1)&=R_{2s}(1)Y_{2s}(1)\\[2ex]\varphi_{2s}(2)&=R_{2s}(2)Y_{2s}(2)\end{aligned}\right\}$$

…(A.2.32)

After integrated over all spins in equation (A.2.31) and substituted equation (A.2.32) into (A.2.31) we get:

$$\Gamma_{34}'(spinless) = \left[R_{2s}(1)Y_{2s}(1)R_{2s}(2)Y_{2s}(2)\right]^2 \qquad \text{….(A.2.33)}$$

now we can integrate over all angular part to get:

$$\Gamma'_{34}(1,2) = R_{2s}{}^2(1)R_{2s}{}^2(2) \qquad \text{…(A.2.34)}$$

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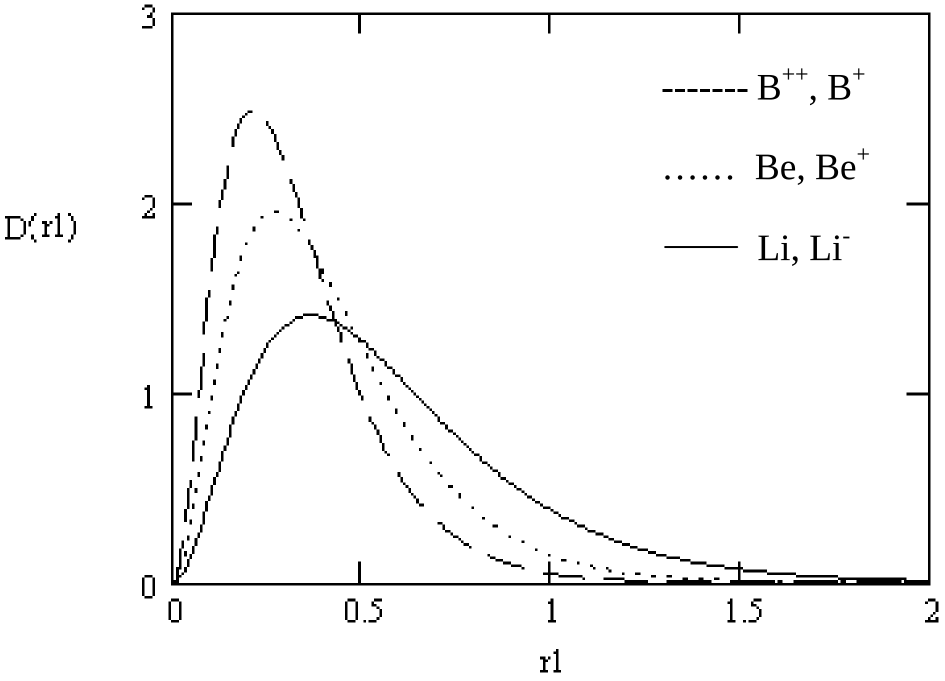

Figure (3-1) variation of one particle radial densities for the K-shell of Li-like ions (Li, Be^{+}, B^{++}) and Be-like ions (Li^{-}, Be, B^{+}).

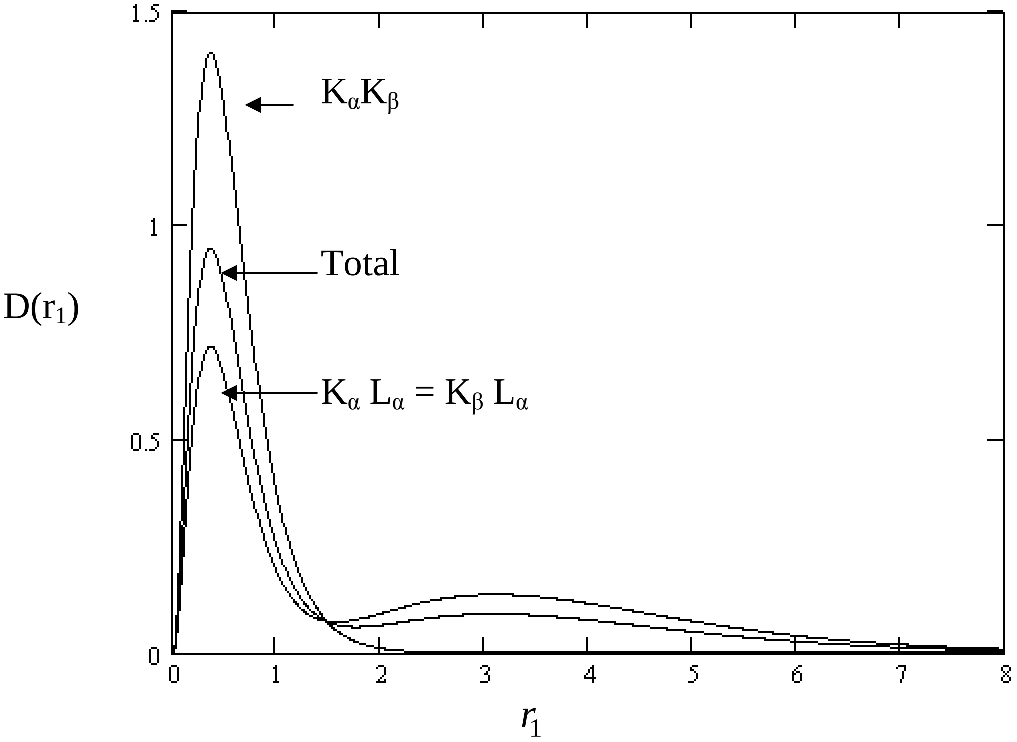

Figure (3-2) variation of the individual shells and the total of the one particle radial density for the Li atom.

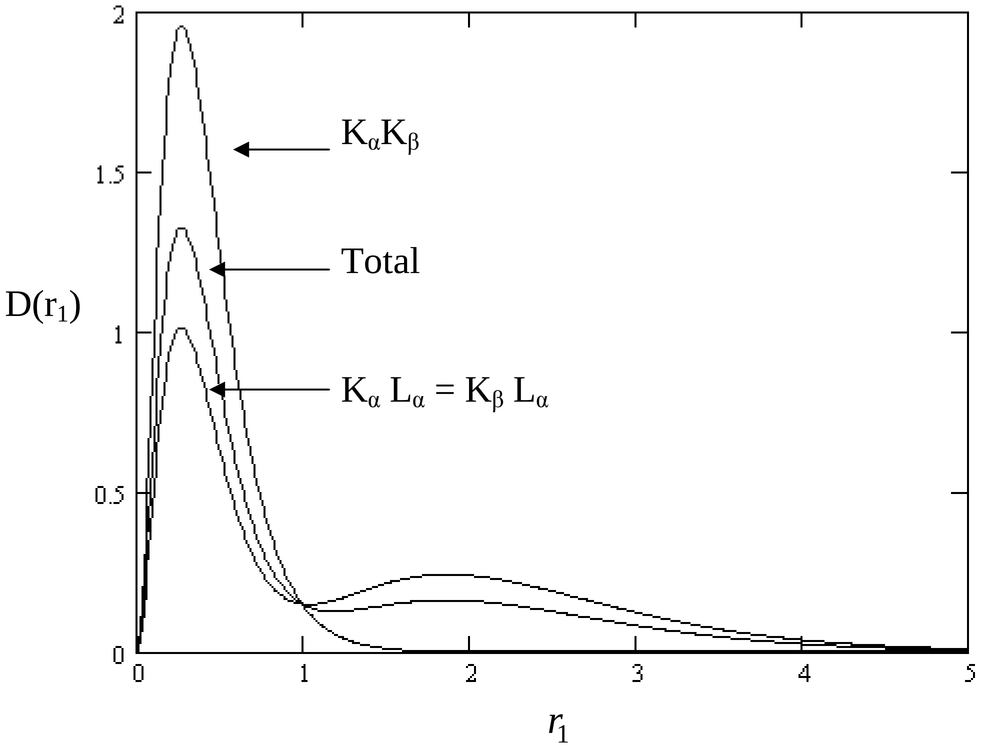

Figure (3-3) variation of the individual shells and the total of the one particle radial density for the Be^+ ion.

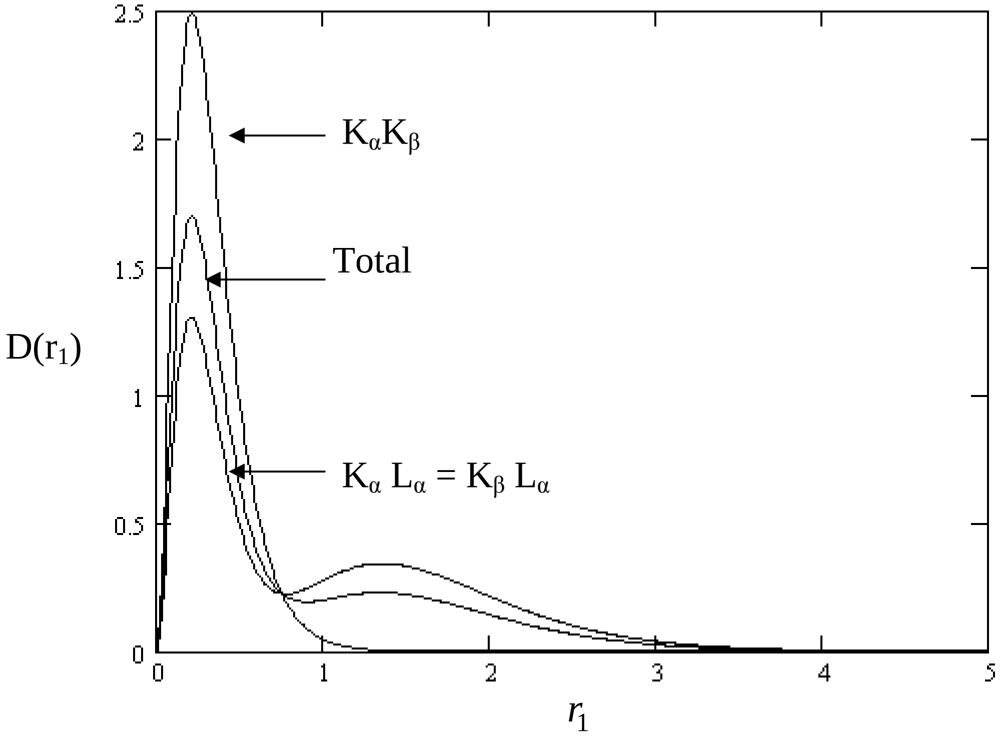

Figure (3-4) variation of the individual shells and the total of the one particle radial density for the B^{++} ion.

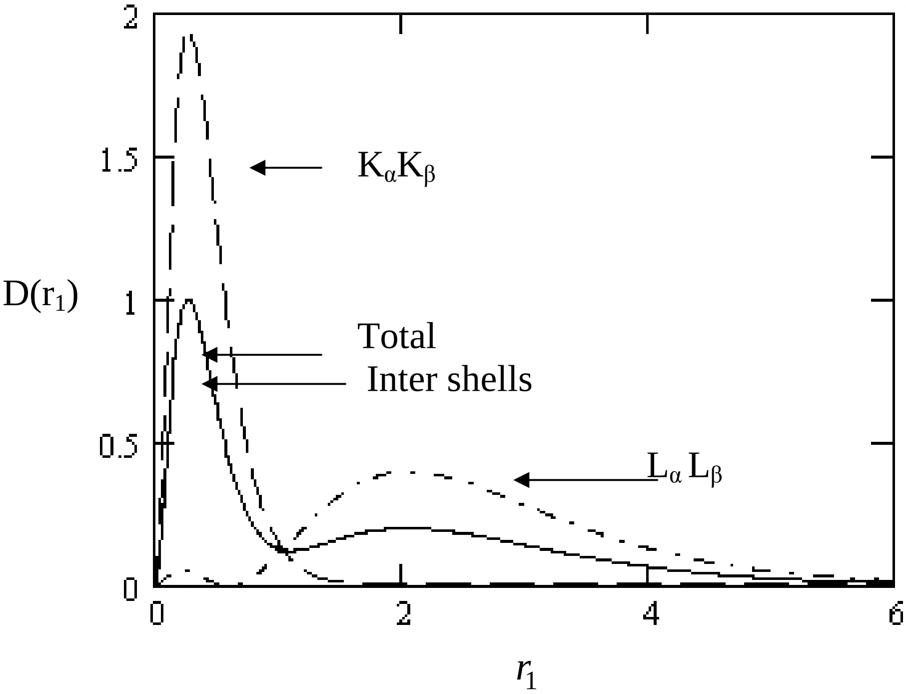

Figure (3-5) variation of the individual shells and the total of the one particle radial density for the Li⁻ ion.

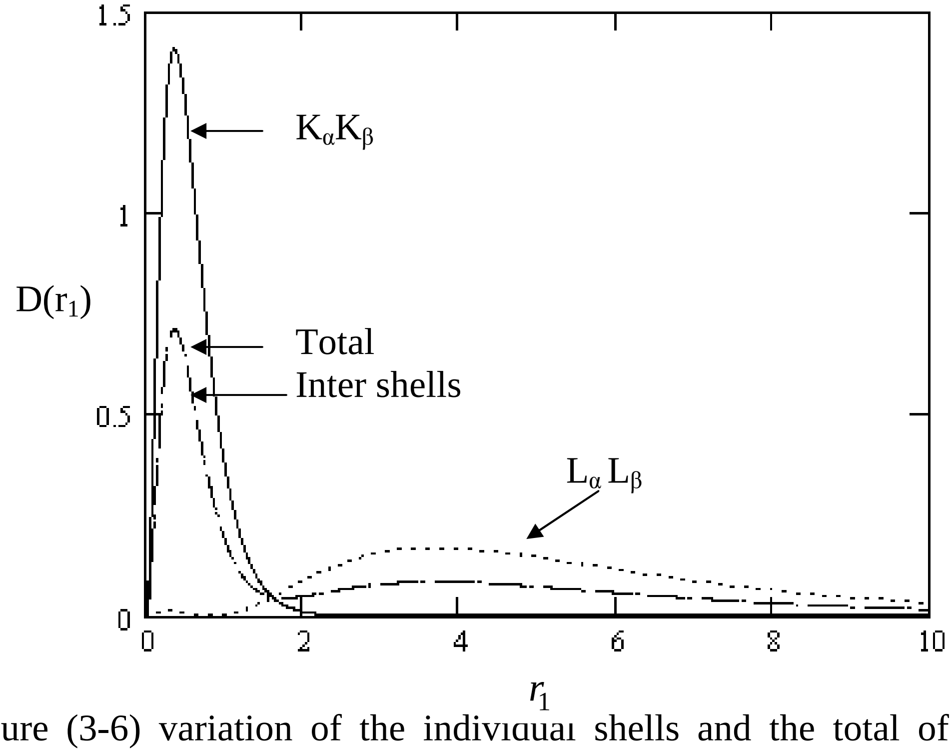

Figure (3-6) variation of the individual shells and the total of the one particle radial density for the Be atom.

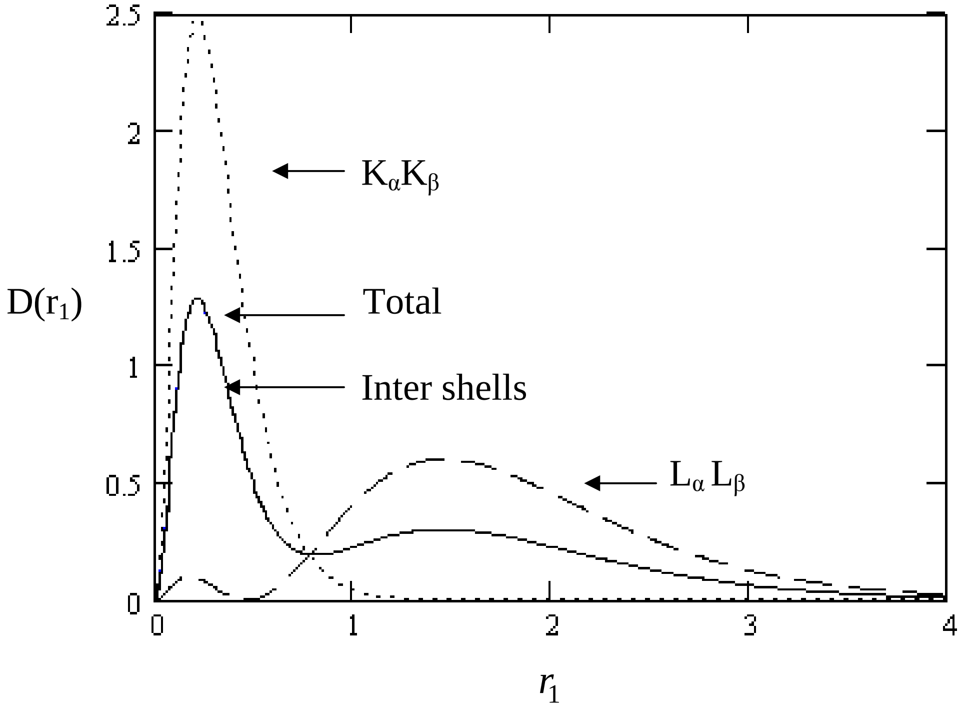

Figure (3-7) variation of the individual shells and the total of the one particle radial density for the B^+ ion.

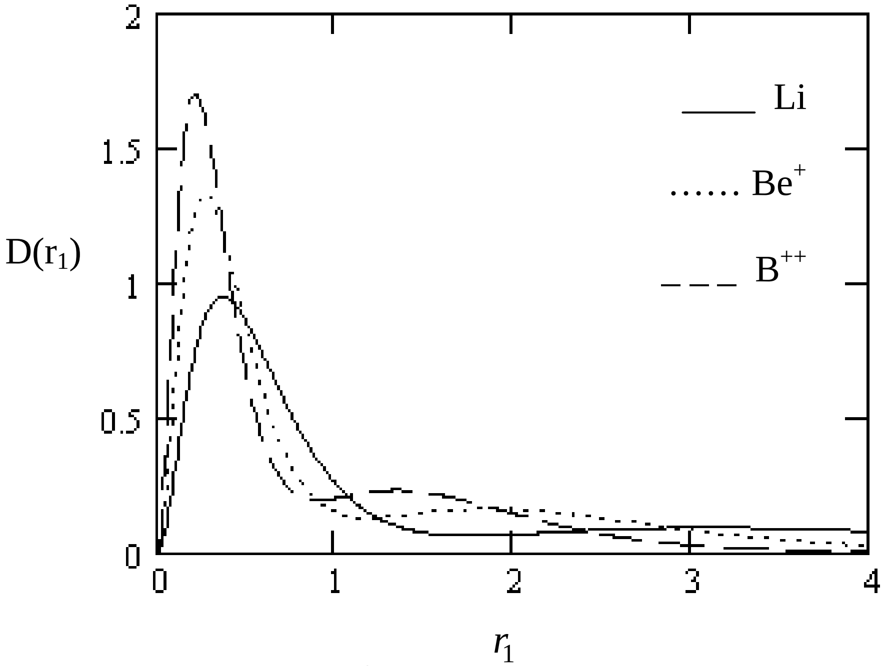

Figure (3-8) variation of the total one particle radial densities of Li-like ions (Li, Be^+, B^{++}).

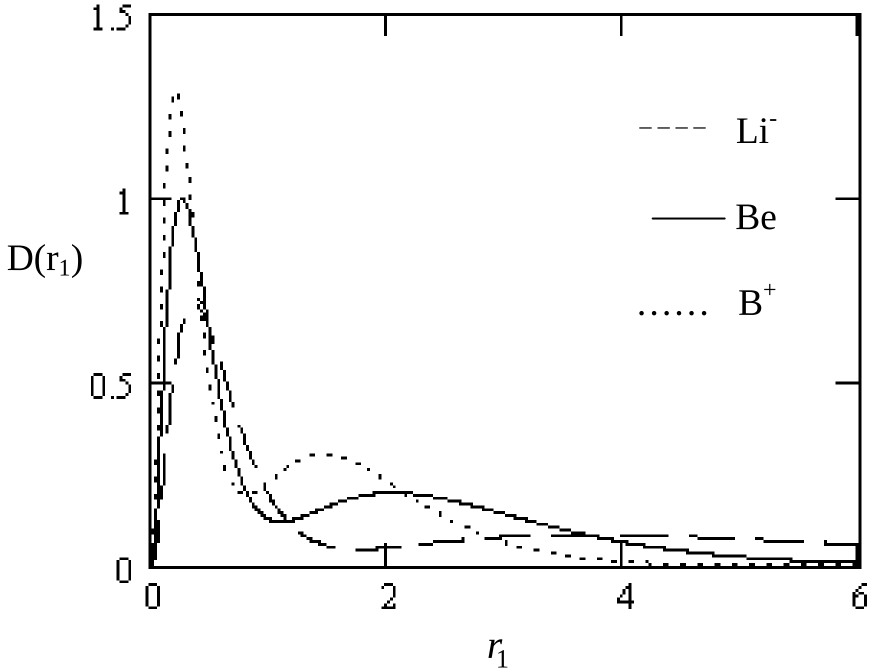

Figure (3-9) variation of the total one particle radial densities of Be-like ions (Li$^-$, Be, B$^+$).

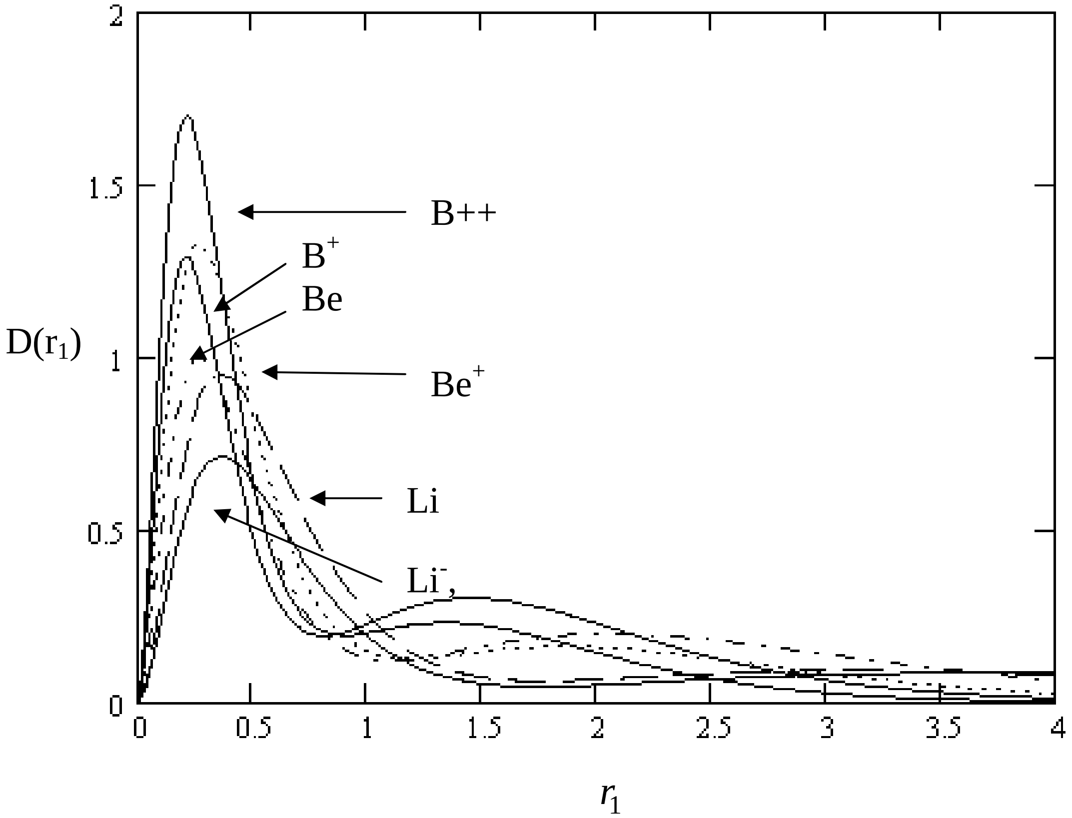

Figure (3-10) variation of the total one particle radial densities of Li-like ions (Li, Be$^+$, B^{++}) and for Be-like ions (Li$^-$, Be, B$^+$).

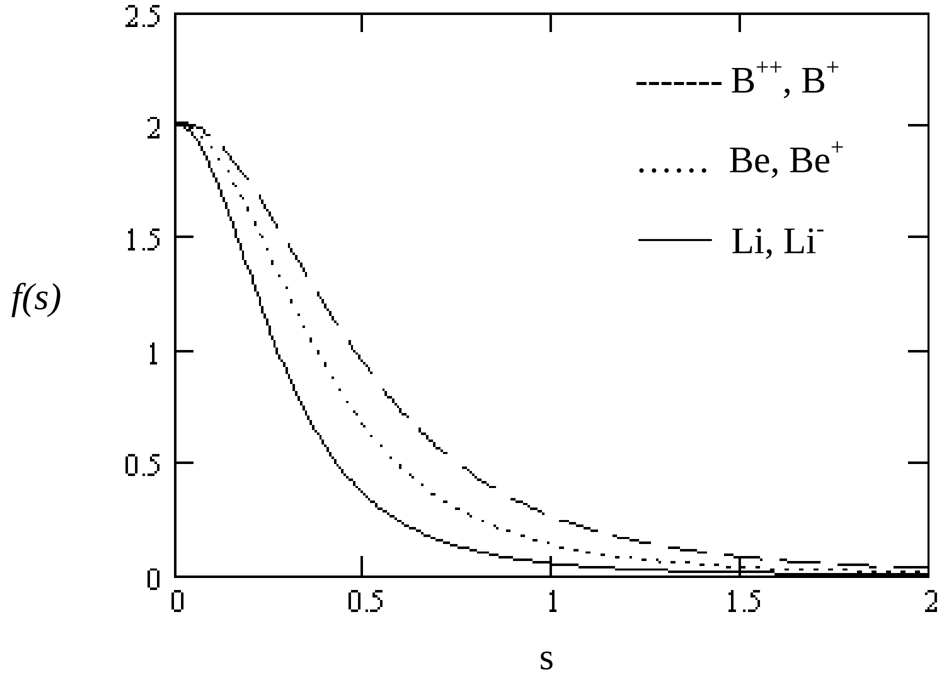

Figure (3-11) variation of scattering form factor with s for the K-shell of Li-like ions (Li, Be^+, B^{++}) and Be-like ions (Li^-, Be, B^+).

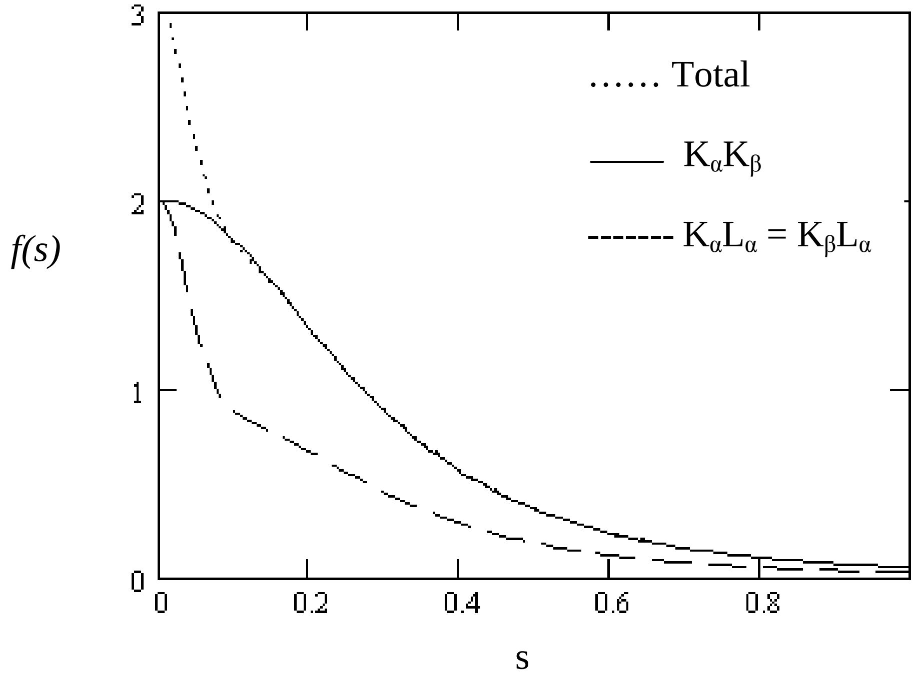

Figure (3-12) variation of the individual shells and the total scattering form factors with s for Li atom.

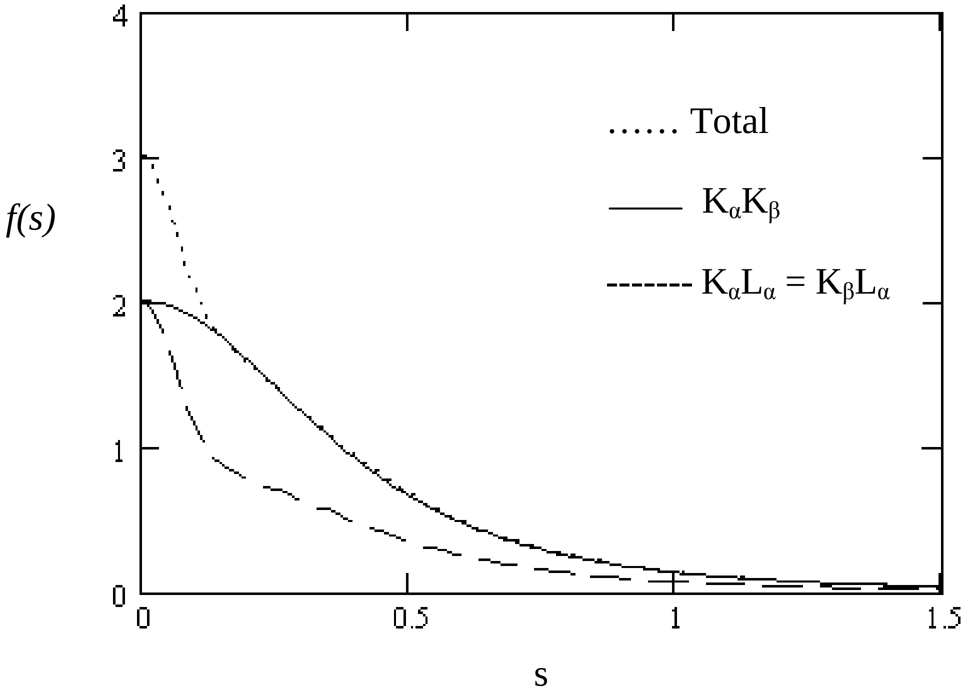

Figure (3-13) variation of the individual shells and the total scattering form factors with s for Be^+ ion.

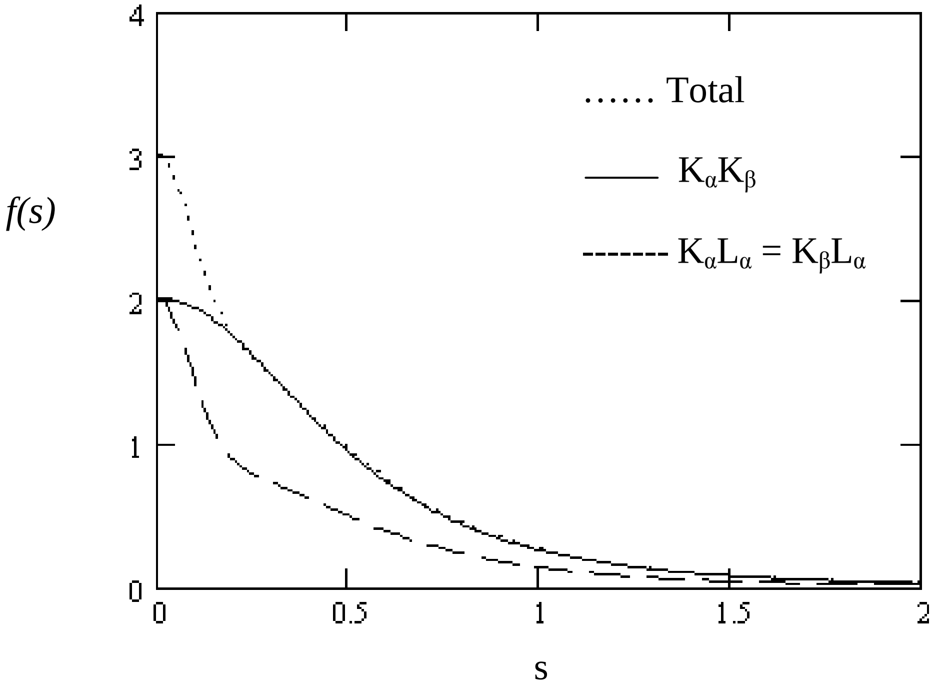

Figure (3-14) variation of the individual shells and the total scattering form factors with s for B^{++} ion.

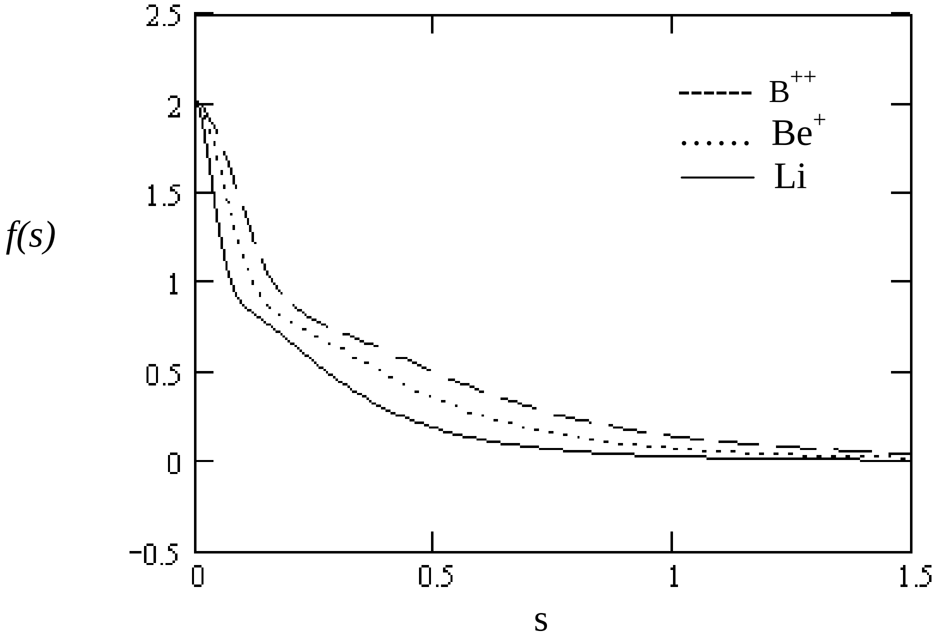

Figure (3-15) variation of the inter shells scattering form factor with s for Li-like ions (Li, Be^{+}, B^{++}).

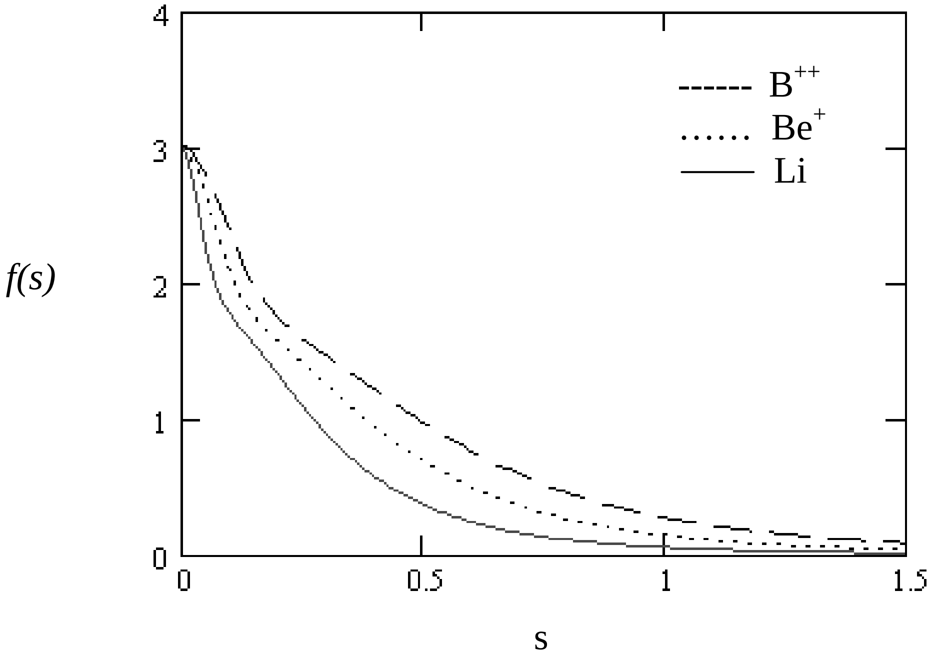

Figure (3-16) variation of the total scattering form factor with s of Li-like ions (Li, Be^{+}, B^{++}).

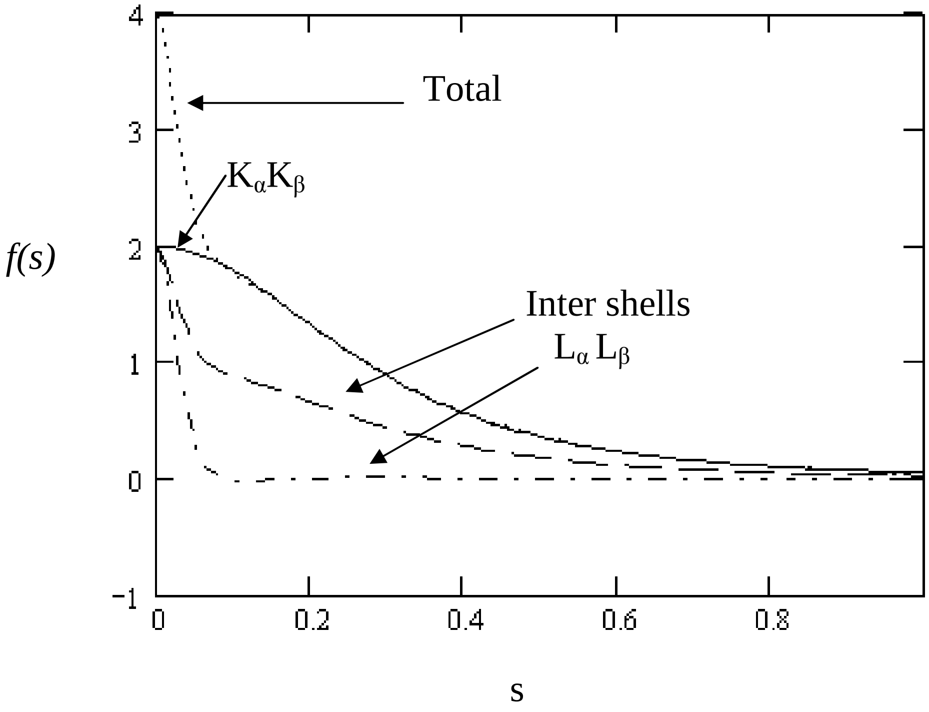

Figure (3-17) variation of the individual shells and the total scattering form factors with s for Li^- ion.

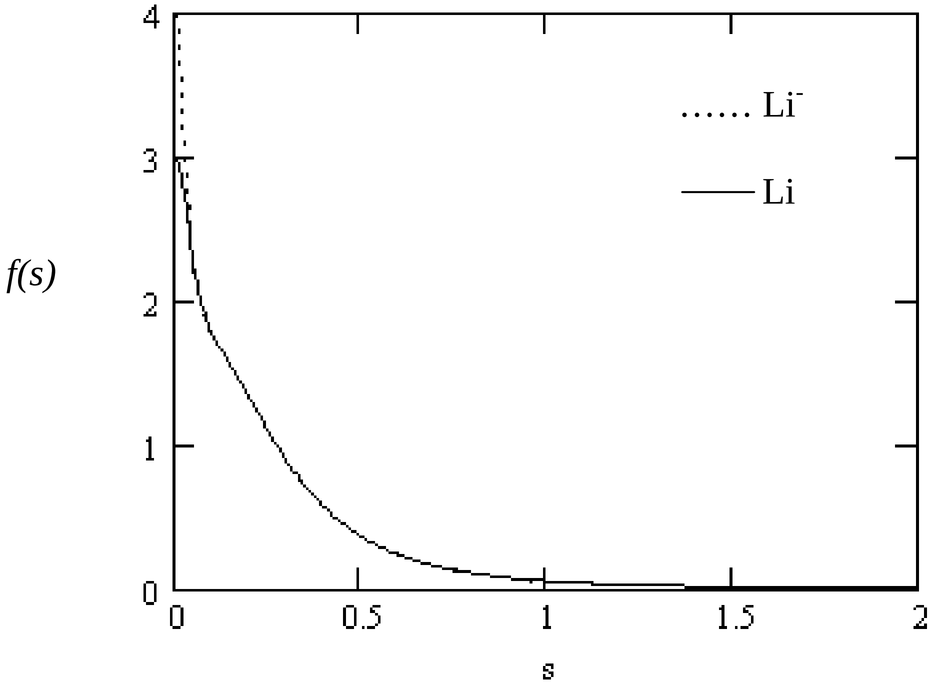

Figure (3-18) variation of the total scattering form factor with s for Li atom and Li^- ion.

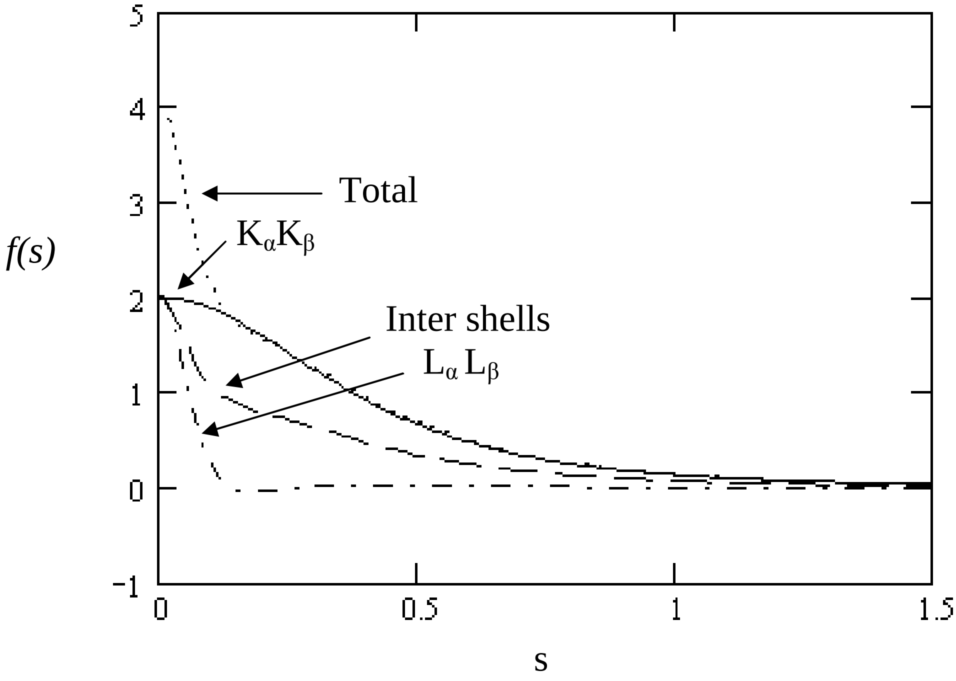

Figure (3-19) variation of the individual shells and the total scattering form factors with s for Be ion.

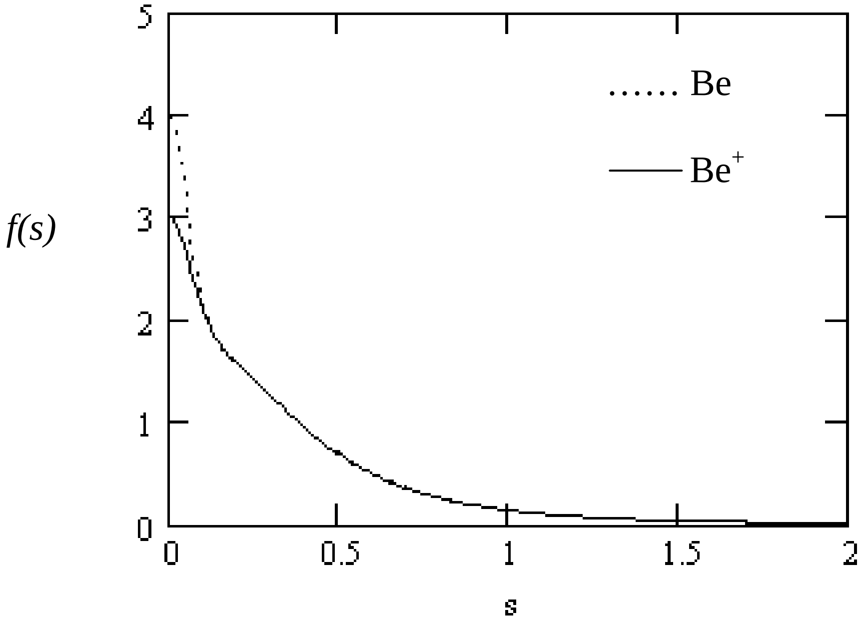

Figure (3-20) variation of the total scattering form factor with s for Be atom and Be^+ ion.

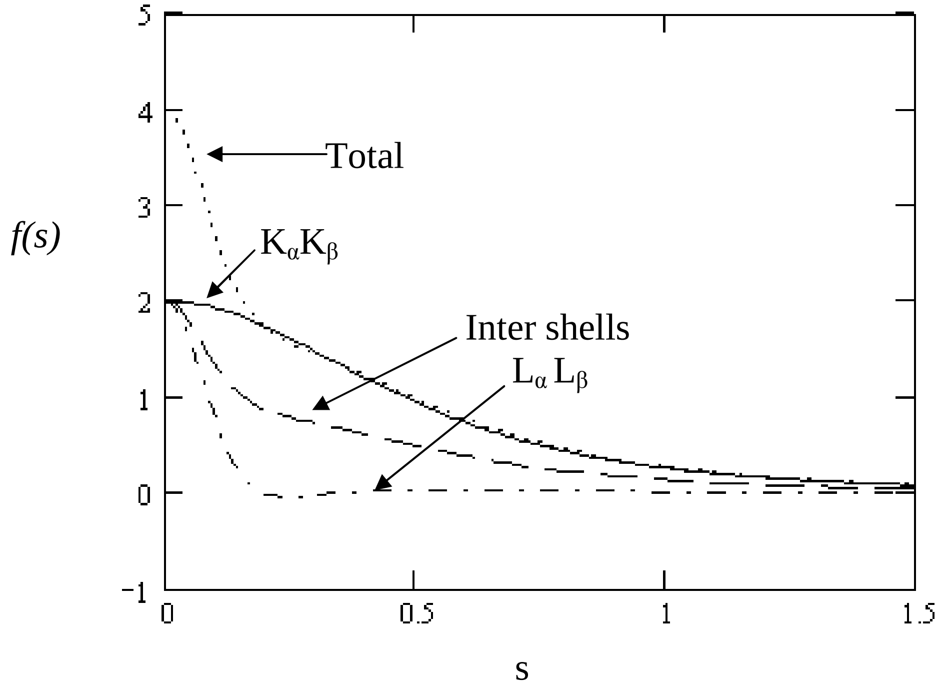

Figure (3-21) variation of the individual shells and the total scattering form factors with s for B^+ ion.

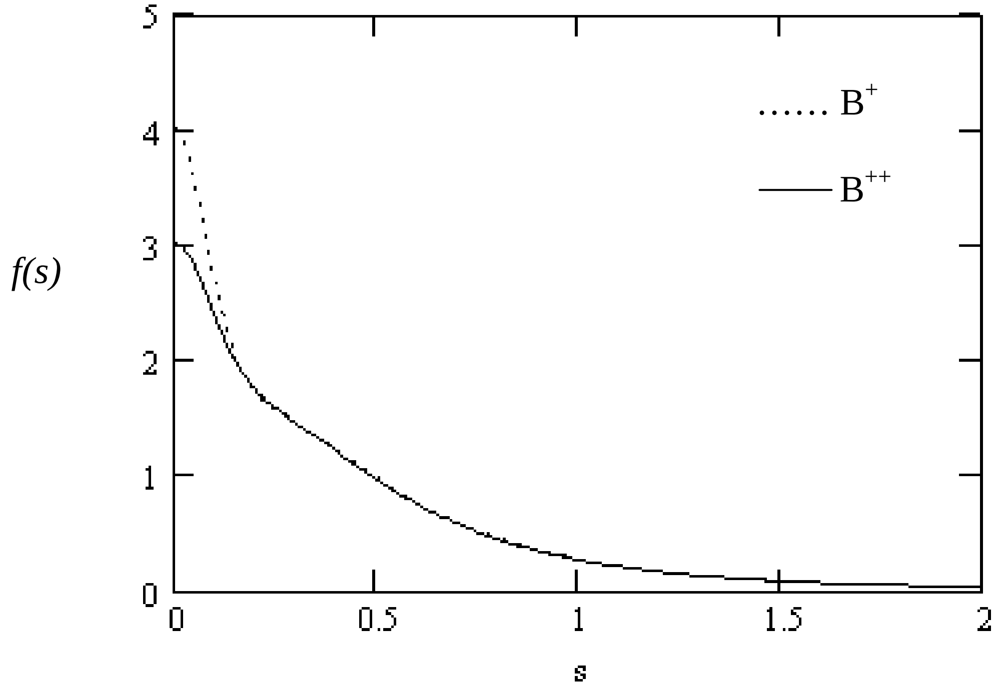

Figure (3-22) variation of the total scattering form factor with s for B^+ ion and B^{++} ion.

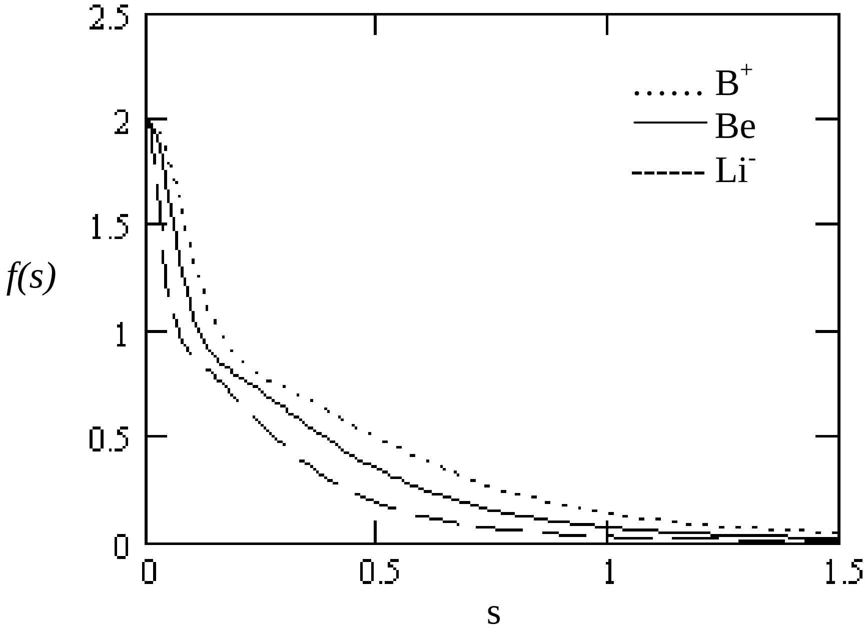

Figure (3-23) variation of the inter shells scattering form factor with s for Be-like ions (Li^{-}, Be, B^{+}).

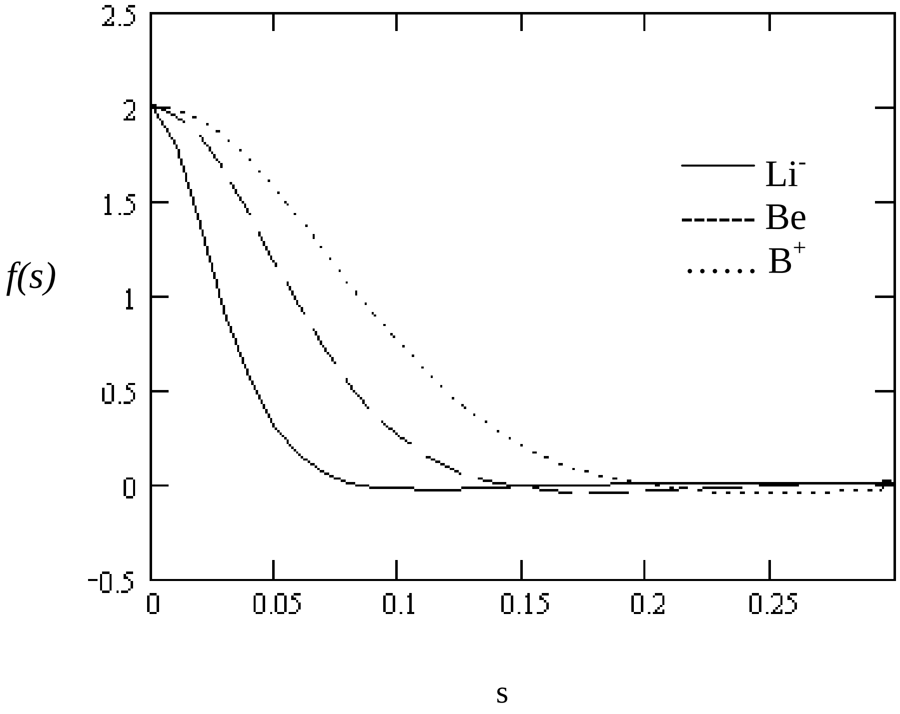

Figure (3-24) variation of L_{α} L_{β} shells scattering form factor with s for Be-like ions (Li^{-}, Be, B^{+}).

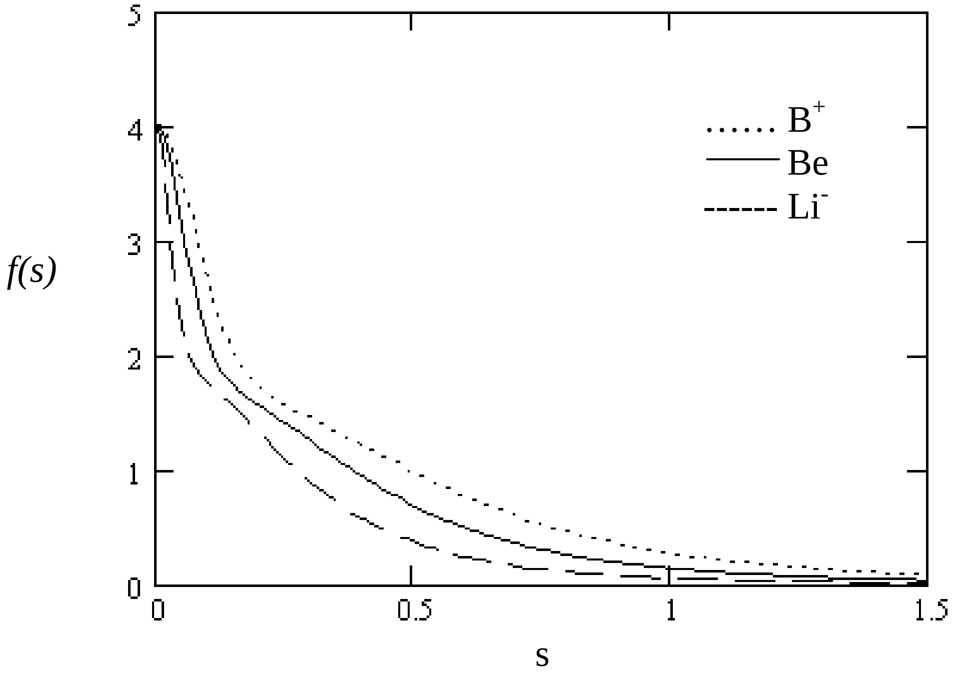

Figure (3-25) variation of the total scattering form factor with s of Be-like ions (Li$^-$, Be, B$^+$).

Table (3-1) data for Li atom.[53]

Li				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	4.3069	0.141279	-0.022416
1	0	2.4573	0.874231	-0.135791
3	0	6.7850	-0.005201	0.000389
2	0	7.4527	-0.002307	-0.000068
2	0	1.8504	0.006985	-0.076544
2	0	0.7667	-0.000305	0.340542
2	0	0.6364	0.000760	0.715708

Table (3-2) data for Be^+ ion.[47]

Be^+				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	4.0	0.91711	-0.19922
3	0	1.081	-0.00129	0.00045
3	0	4.68	0.07960	-0.01081
3	0	3.40	0.04314	0.00728
3	0	1.97	-0.00331	0.42943
3	0	1.31	0.00178	0.61599

Table (3-3) data for B^{++} ion.[47]

B^{++}				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	5.0	0.93299	-0.23270
3	0	12.0	-0.00151	0.00050
3	0	5.97	0.06390	-0.00787
3	0	4.28	0.03661	0.00451
3	0	2.70	0.00409	0.42344
3	0	1.863	0.00192	0.62350

Table (3-4) data for Be atom.[53]

Be				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	5.7531	0.285107	-0.016378
1	0	3.7156	0.474813	-0.155066
3	0	9.9670	-0.001620	0.000426
3	0	3.7128	0.052852	-0.059234
2	0	4.4661	0.243499	-0.031925
2	0	1.2919	0.000106	0.387968
2	0	0.8555	-0.000032	0.685674

Table (3-5) data for B^+ ion.[56]

B^+				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	4.42994	0.92801	-0.20288
1	0	7.86336	0.08063	-0.01942
2	0	1.58241	0.0032	0.7349
2	0	4.01022	-0.00081	-0.09218
2	0	1.25021	-0.00198	0.34527

Table (3-6) data for Li^- ion.[56]

Li^-				
n	ℓ	ζ	C_{1s}	C_{2s}
1	0	2.47472	0.89760	-0.10034
1	0	4.69209	0.11212	-0.01100
2	0	0.26763	-0.00003	0.39768
2	0	0.53399	0.00016	0.56089
2	0	1.01192	-0.00108	0.20478
2	0	1.66285	0.00750	-0.07906

Table (3-7) the maximum and the locations of one particle radial density distribution for the K-shell for Li-like ions (Li, Be^+, B^{++}) and Be-like ions (Li^-, Be, B^+).

	$D(r_1)$ Maximum	Location r_1
Li	1.4057	0.36
Li^-	1.4063	0.36
Be^+	1.9518	0.27
Be	1.9448	0.27
B^{++}	2.4872	0.21
B^+	2.4848	0.21

Table (3-8) the maximum and the locations of one particle radial density distribution for the individual shells and total of Li-like ions (Li, Be^+, B^{++}).

Z	Shell	$D(r_1)$ Maximum	Location r_1
3	$K_\alpha K_\beta$	1.4057	0.36
	$K_\alpha L_\alpha$	0.71658	0.36
		0.13687	3.09
	$K_\beta L_\alpha$	0.71658	0.36
		0.13687	3.09
	Total	0.94629	0.36
		0.091246	3.09
4	$K_\alpha K_\beta$	1.9518	0.27
	$K_\alpha L_\alpha$	1.0112	0.26
		0.242	1.86
	$K_\beta L_\alpha$	1.0112	0.26
		0.242	1.86
	Total	1.3247	0.27
		0.16133	1.86
5	$K_\alpha K_\beta$	2.4872	0.21
	$K_\alpha L_\alpha$	1.3014	0.21
		0.34302	1.35
	$K_\beta L_\alpha$	1.3014	0.21
		0.34302	1.35
	Total	1.6967	0.21
		0.22868	1.35

Table (3-9) the maximum and the locations of one particle radial density distribution for the individual shells and total of Li^- ion.

Shell	$D(r_1)$ Maximum	Location r_1
$K_\alpha K_\beta$	1.4063	0.36
$K_\alpha L_\alpha$	0.70977	0.36
	0.084794	3.69
$K_\beta L_\alpha$	0.70977	0.36
	0.084794	3.69
$K_\alpha L_\beta$	0.70977	0.36
	0.084794	3.69
$K_\beta L_\beta$	0.70977	0.36
	0.084794	3.69
$L_\alpha L_\beta$	0.013881	0.3
	0.16958	3.69
Total	0.70977	0.36
	0.084794	3.69

Table (3-10) the maximum and the locations of one particle radial density distribution for the individual shells and total of Be atom.

Shell	$D(r_1)$ Maximum	Location r_1
$K_\alpha K_\beta$	1.9448	0.27
$K_\alpha L_\alpha$	0.99711	0.26
	0.1982	2.05
$K_\beta L_\alpha$	0.99711	0.26
	0.1982	2.05
$K_\alpha L_\beta$	0.99711	0.26
	0.1982	2.05
$K_\beta L_\beta$	0.99711	0.26
	0.1982	2.05
$L_\alpha L_\beta$	0.053109	0.22
	0.39593	2.05
Total	0.99711	0.26
	0.1982	2.05

Table (3-11) the maximum and the locations of one particle radial density distribution for the individual shells and total of B^+ ion.

Shell	$D(r_1)$ Maximum	Location r_1
K_α K_β	2.4848	0.21
K_α L_α	1.2888	0.21
	0.30138	1.45
K_β L_α	1.2888	0.21
	0.30138	1.45
K_α L_β	1.2888	0.21
	0.30138	1.45
K_β L_β	1.2888	0.21
	0.30138	1.45
L_α L_β	0.09976	0.17
	0.60103	1.46
Total	1.2888	0.21
	0.30138	1.45

Table (3-12) scattering form factor for the K-shell of Li-like ions (Li, Be^+, B^{++}) and for Be-like ions (Li^-, Be, B^+).

$\sin\theta/\lambda$	*f(sinθ/λ)*					
	Li	Be^+	B^{++}	Li^-	Be	B^+
0.0	2	2	2	2	2	2
0.2	1.3208	1.5937	1.7371	1.3211	1.5897	1.7312
0.2*	1.32	1.59	1.73			
0.4	0.5617	0.9189	1.1918	0.5619	0.9160	1.1903
0.4*	0.56	0.918	1.19			
0.6	0.2333	0.4763	0.7279	0.2334	0.4747	0.7276
0.6*	0.233	0.476	0.72			
0.8	0.1060	0.2491	0.4309	0.1060	0.2485	0.4307
0.8*	0.106	0.249	0.43			
1	0.0531	0.1366	0.2581	0.0531	0.1364	0.2580
1*	0.053	0.136	0.25			

* ref.[33]

Table (3-13) scattering form factor of the total and the individual shells for the Li atom.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$			
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	Total
0.0	2	2	2	3
0.2	1.3208	0.6640	0.6640	1.3245
0.4	0.5617	0.2883	0.2883	0.5692
0.6	0.2333	0.1196	0.1196	0.2363
0.8	0.1060	0.0544	0.0544	0.1074
1	0.0531	0.0274	0.0274	0.0540

Table (3-14) scattering form factor of the total and the individual shells for the for the Be^+ ion.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$			
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	Total
0.0	2	2	2	3
0.2	1.5937	0.7732	0.7732	1.5701
0.4	0.9189	0.4775	0.4775	0.9370
0.6	0.4763	0.2503	0.2503	0.4885
0.8	0.2491	0.1310	0.1310	0.2556
1	0.1366	0.0718	0.0718	0.1401

Table (3-15) scattering form factor of the total and the individual shells for the for the B^{++} ion.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$			
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	Total
0.0	2	2	2	3
0.2	1.7371	0.8775	0.8775	1.7461
0.4	1.1918	0.6079	0.6079	1.2038
0.6	0.7279	0.3859	0.3859	0.7500
0.8	0.4309	0.2301	0.2301	0.4456
1	0.2581	0.1382	0.1382	0.2673

Table (3-16) scattering form factor of the total and the individual shells for the for the Li^- ion.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$						
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	$K_\alpha L_\beta$	$K_\beta L_\beta$	$L_\alpha L_\beta$	Total
0.0	2	2	2	2	2	2	4
0.2	1.3211	0.6626	0.6626	0.6626	0.6626	0.0040	1.3252
0.4	0.5619	0.2845	0.2845	0.2845	0.2845	0.0070	0.5690
0.6	0.2334	0.1182	0.1182	0.1182	0.1182	0.0030	0.2364
0.8	0.1060	0.0536	0.0536	0.0536	0.0536	0.0012	0.1072
1	0.0531	0.0266	0.0266	0.0266	0.0266	0.0002	0.0533

Table (3-17) scattering form factor of the total and the individual shells for the for the Be atom.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$						
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	$K_\alpha L_\beta$	$K_\beta L_\beta$	$L_\alpha L_\beta$	Total
0.0	2	2	2	2	2	2	4
0.2	1.5897	0.7773	0.7773	0.7773	0.7773	-0.0351	1.5546
0.4	0.9160	0.4709	0.4709	0.4709	0.4709	0.0258	0.9419
0.6	0.4747	0.2460	0.2460	0.2460	0.2460	0.0171	0.4919
0.8	0.2485	0.1288	0.1288	0.1288	0.1288	0.0091	0.2576
1	0.1364	0.0707	0.0707	0.0707	0.0707	0.00495	0.1414

Table (3-18) scattering form factor of the total and the individual shells for the for the B^+ ion.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$						
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$	$K_\beta L_\alpha$	$K_\alpha L_\beta$	$K_\beta L_\beta$	$L_\alpha L_\beta$	Total
0.0	2	2	2	2	2	2	4
0.2	1.7312	0.8614	0.8614	0.8614	0.8614	-0.0085	1.7228
0.4	1.1903	0.6060	0.6060	0.6060	0.6060	0.0216	1.2119
0.6	0.7276	0.3814	0.3814	0.3814	0.3814	0.0353	0.7629
0.8	0.4307	0.2271	0.2271	0.2271	0.2271	0.0234	0.4542
1	0.2580	0.1361	0.1361	0.1361	0.1361	0.01410	0.2722

Table (3-19) Comparison the total energy.

	Present work	Other works	
Li	-7.4327	Ref.[53]	-7.4327
Be^+	-14.277	Ref.[47]	-14.277
B^{++}	-23.37	Ref.[47]	-23.37
Li^-	-7.428	Ref.[56]	-7.42
Be	-14.5730	Ref.[53]	-14.5730
B^+	-24.237	Ref.[56]	-24.237

1.1 Mechanism of x-ray Production

Many of electrons that strike matter do nothing spectacular at all. Most of them undergo glancing collisions with the particles of the matter, and in the course of these collisions the electrons loss their energy a little at a time and thus merely increase the average kinetic energy of the particles in the material. The result is that the temperature of the target material is increased. It is found that most of the energy of the electron beam goes into heating the target. Some of the bombarding electrons make solid hits and lose most or all of their energy in just one collision. These electrons are rapidly decelerated. When an electron loses a large amount of energy by being decelerated, an energetic pulse of electromagnetic radiation is produced. This is an inverse photoelectric effect in which an electron produces a photon. It is found that electrons of a given energy produce x-ray photons with a certain maximum energy. Both effects confirm the quantum view of radiation.

Looking at the collision process more closely, however, it is found another very important kind of collision energy exchange. The bombarding electron may also give energy to electrons bound to the target atoms. If these atomic electrons are freed from their home atoms, ions are produced. Since x-ray producing electrons have energies of the order of many thousands of electrons volts, it is very easy for them to produce ions by removing outer electrons. x-ray producing electrons may also have enough energy to produce ions by removing inner electrons from the atom, even down to the inner most or K-shell. Such an ion has a low-energy hole in its electronic structure, and this vacancy is promptly filled when one of its electrons in a higher energy state falls to this low-energy level. When an outer electron falls into such a vacancy, it will radiate a photon of this energy. Such photons are in the x-ray region and have wave lengths which are fractions of angstroms. This mechanism, which accounts for a significant part of x-ray production, produces x-rays having particular wave lengths which are characteristic of the target material. [1]

1.2 The Scattering

When an electromagnetic wave impinges on a small body, the charged particles within the body experience forces due to the wave fields and are set into oscillatory motion. They therefore radiate, in accordance with the oscillating multipole moments set up in the body. The result is that energy is extracted from the incident wave and sent out in some angular distribution over the entire 4π solid angle around the body. This is called scattering. [2]

1.3 Scattering of x-rays

When abeam of x-rays passes through a substance, the electrons in this substance are set into vibration and radiate x-rays in all directions. The radiation emitted by these electrons is called scattered or secondary radiation. [3]

1.4 The x-ray Form Factor

Atoms are not mere mathematical points in space but possess finite sizes which are of the same magnitude as the x-ray wave lengths used in diffraction studies. Moreover, the electrons are spread throughout the volume of the atom, with the result that not all of them can be expected to scatter in phase.

Consider Figure (1-1) in which, for simplicity, the electrons are shown as points arranged around the central nucleus. The wave scattered in the forward direction by electrons A and B are exactly in phase on a wave front such as XX', because each wave has traveled the same distance before scattering.

The other scattered waves shown in the figure, however, have a path difference equal to (CB-AD) and thus somewhat out of phase along a wave front such as YY', the path difference being less than one wave length [4,5]. Partial interference occurs between the wave scattered by A and B, with the result that the net amplitude of the wave scattered in this directions is less than that of the wave scattered by the same electrons in the forward direction.

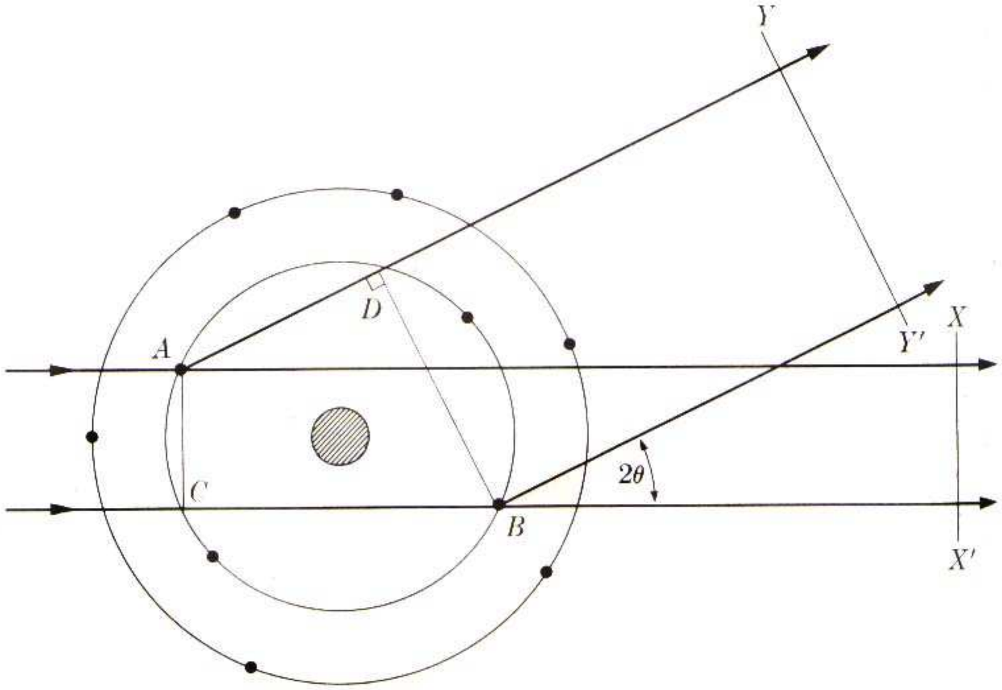

Figure (1-1) X-ray scattering by an atom [5]

A quantity *f(s)*, the atomic scattering factors, is used to describe the "efficiency" of scattering of a given atom in a given direction, which is defined as a ratio of amplitudes [5,6]

$$f(s) = \frac{Amplitude\ of\ the\ wave\ scattered\ by\ an\ atom}{Amplitude\ of\ the\ wave\ scattered\ by\ one\ electron}$$ … (1-1)

From what has been said already, it is clear that *f(s)* equal to the number of electros for any atom scattering in the forward direction.

For the scattering angle θ increases, however, the waves scattered by individual electrons become more and more out of phase and *f(s)* decreases.

The atomic scattering factor depends also on the wave lengths of the incident beam:

As a fixed value of θ, *f(s)* will be smaller for the shorter wave lengths, since the path differences will be larger relative to the wave length, leading to greater interference between the scattered beams.

The scattering factor is sometimes called the form factor, because it depends on the way in which the electrons are distributed around the nucleus.

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 (see appendix 1) [5]:

$$f(s) = \int_0^\infty D(r) \frac{\sin 4\pi sr}{4\pi sr} dr$$ … (1-2)

Where: $4\pi s$ is called the momentum transfer, $\frac{\sin sr}{sr}$ is the spherical Bessel function of zero order [7], and $S = \sin\theta / \lambda$

Since:

$$J_n = x^n \left(\frac{-1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right)$$ … (1-3)

The form factor $f(s)$ is related to the incoherent scattering function $S(s)$ by the following relationship [8]:

$$S(s) = N + 2\int_0^\infty f(r_{12})\frac{\sin sr_{12}}{sr_{12}}dr_{12} - |f(s)|^2 \qquad \text{… (1-4)}$$

Where $f(r_{12})$ is the electron-electron distribution function for each shell, and N is the atomic charge.

In solids, the calculations of x-ray scattering factors have always been based on the assumption that the total charge density can be approximated as a sum of atomic charge distributions on each lattice site. The total scattering factor $f(s)$ is then a sum of atomic scattering factors f_n multiplied by appropriate phase factors:

$$f(S) \cong \sum_n f_n e^{-i\vec{S}.\vec{r}_n} \qquad \text{…(1-5)}$$

Where $\vec{S}$ is a reciprocal lattice vector and $\vec{r}_n$ the position of the nth atom in the unit cell [8].

1 .5 Physical Importance of Atomic Form Factor

The functions $f(s)$ and $S(s)$ play important role in the theory of scattering of x-rays and electrons by atoms as follows:

1- The total incoherent scattering cross section σ_{inch} of the photon by an atom [9, 10].

$$\sigma_{inch} = \frac{1}{2}r_0^{\ 2}(1+\cos^2\theta)^2 ZS(s) \qquad \text{… (1-6)}$$

2- The differential cross-section $\frac{d\sigma_{el}}{d\Omega}$ for the elastic scattering of electrons by an atom.

$$\frac{d\sigma_{el}}{d\Omega} = \frac{4a_0^{\ 2}}{(ka_0)^4}\left|Z - f(s)\right|^2 \qquad \text{… (1-7)}$$

Where $a_0 = \hbar^2 / m_e e^2$ is the Bohr radius.

In this case, We may interpret $f(s)$ as representing the effective shielding of the nuclear charge Z [9].

3- The nuclear magnetic shielding constant σ_d [11,12].

$$\sigma_d = \frac{2\alpha^2}{3\pi}\int_0^\infty f(s)ds \qquad \text{…(1-8)}$$

Where: $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant and it is equal to

(7.297353*10^{-3}) [13].

4- The coherent scattering intensity, which is related to the square absolute form factor as:[14,15,16]

$$\frac{I_{coh}}{I_{cl}} = \left| f(s)\right|^2 \qquad \text{…(1-9)}$$

where:

I_{cl} is the classical expression for total intensity of radiation scattered by a free electron initially at rest.

5- The total scattering intensity, which is related to the square absolute form factor and incoherent scattering function as [17]:

$$\frac{I_{tot}}{I_{cl}} = S(s) + \left| f(s)\right|^2 \qquad \text{…(1-10)}$$

6- The differential cross-section $\frac{d\sigma_{inel}}{d\Omega}$ of electrons summed over all inelastic collisions with an atom , when the momentum of the incident electron is very large compared to the momentum transfer ,is [9]:

$$\frac{d\sigma_{inel}}{d\Omega} = 4a_0^{\ 2}/(ka_0)^4\, ZS(s) \qquad \text{… (1-11)}$$

7- The Geometrical structure factor $F(hkl)$ which is related with the form factor by:

$$F(hkl)=\sum_{n=1}^{N} f(s)e^{i\phi_n} \qquad \ldots(1\text{-}12)$$

Where:

ϕ_n is the phase difference, and *(hkl)* is called Miller indices

To summarize, when a monochromatic beam of x-rays strikes an atom, two scattering process occur. Tightly bound electrons are set into oscillation and radiate x-rays of the same wavelength as that of the incident beam. More loosely bound electrons scatter part of the incident beam and slightly increase its wavelength in the process.

1.6 Historical Review

Freeman and *Wood* (1958) calculated an atomic scattering factor for iron by using self consistent field wave functions [18].

Silverman and *Obta* (1962) have derived two sum rules relating coherent x-ray scattering data to the diamagnetic nuclear shielding constant and to the self-energy of the charge distribution of the scattering [19].

RUSIGI and *Tiwari* (1963) calculate the nuclear magnetic shielding constants and x-ray atomic scattering factor for two, three, and four electron systems using the best analytical self-consistent field functions of Roothaan, Sachs, and Weiss, and compared the reported values with the ones already published [20].

Chipman and *Jennings* (1963) have calculated the atomic scattering factor of Ne, Ar, Kr, and Xe by using Hartree- fock wave function and compared the results with the experimental values [21].

Bartell and *Gavin* (1964) have studied the effects of electron correlation in x-ray and electron diffraction from the comparison of elastic and inelastic scattering factors, which were calculated from Hartree-Fock wave functions and from wave functions explicitly including electron correlation [22].

Bartell and *Gavin* (1965) have calculated the electron-electron and electron-nuclear radial distribution function of $f(r_{12})$ and $D(r)$ for ground states of helium like systems (Z=2 to 8) by using correlated and un correlated wave functions published by Roothaan et al, and calculated elastic and inelastic scattering factors [16].

Chattar and *Swamy* (1966) have estimated the relativistic effects in x-ray scattering form factors from Xenon and compared the results with Hartree-Fock values and experimental measurements [23].

Frank and *Arlinghaus* (1967) have calculated the crystal charge density for copper and aluminum and used it to find the scattering factors by using the augmented-plain-wave method. These factors were compared with those determined from Hartree-Fock atomic calculations [24].

Banyard (1968) has analyzed and compared five wave functions for H^-, and he studied the two-particle radial density $D(r1,r2)$and the one particle radial density $D(r1)$ for the coherent x-ray scattering contribution $f(s)$ and the $< r^k >$ where $-2 \leq k \leq 2$ [25].

Kim and *Inokuti* (1968) have calculated the atomic form factor and the incoherent-scattering function of the helium atom from several wave functions of differing accuracies. The form factor calculated from the Hartree-Fock wave function is in very close agreement with that from the 20-term Hylleraas wave function for all values of the momentum transfer. The incoherent-scattering calculated from the correlated wave functions, gives values at small momentum transfers, approximately 5% lower than that of the Hartree-Fock wave function [9].

Banyard and *Baker* (1969) have studied the electron correlation in an iso electronic series possessing electrons with anti parallel spins, H^-, *He*,

and Li^+. They have used three wave functions, two introduce correlation, one by configuration interaction, the other by including Hylleraas-type correlation factors and the third function was based on the Hartree-Fock approach. The correlation within the wave function is demonstrated by presenting two-particle density difference maps $\Delta D(r1,r2)$ relative to the uncorrelated approach, and graphs of the radial density $D(r)$.
The coherent x-ray scattering contribution $f(s)$, and $< r^n>$ results are compared throughout with those from a more accurate wave function [26].

Benesch and *Smith* (1970) determined correlated x-ray scattering factors for the ^2S ground state of the Lithium atom and correlated electron scattering amplitudes are also obtained with in the firs Bohr approximation. For purposes of comparison, scattering factors were computed from various independent particle model wave functions [15].

Brown (1970) calculated the atomic form factors and incoherent-scattering functions for helium isoelectric sequence through Z=10 with correlated ground-state wave functions. The results compared with published accurate calculations for helium [27].

Brown (1971) calculated the atomic form factors and incoherent-scattering functions for the lithium and beryllium isoelectric sequence through Z=8 with correlated ground-state wave functions [28].

Singh and *Smith* (1971) studied the convergence of the Z-1 expansion of the nuclear magnetic shielding constant σ and the x-ray form factors $f(s)$ within the Hartree-Fock approximation for the ground state of two-, three-, four- electrons of atoms and ions [29].

Benesch et al (1972) have studied the convergence of the Z-1 expansion of the nuclear magnetic shielding constant and the x-ray form factor $f(s)$ and total scattered x-ray intensities from explicitly correlated wave functions and then applied to such wave function recently constructed for the ground state of He-like ions from H^- through Mg^{+10} [30].

Thakkar and *Smith* (1978) have derived the integral formula necessary to compute x-ray intensities from explicitly correlated wave functions and then applied to such wave function recently constructed for the ground state of He-like ions from H^- through Mg^{+10} [14].

Pucci and *March* (1982) have calculated the scattering form factor *f(s)* for x-ray from atomic ions with atomic ions with classed shells and the $< r^n >$ where $-2 \leq n \leq 2$ for the Ar, Kr, Xe and Kn [31].

Oxley and *Allen* (2000) calculated the atomic scattering factors for K-shell ionization for elements in the range Z=6 (Carbon) to Z=50 (Tin) and for L-shell ionization in the range Z=20 (calcium) to Z=60 (Neodymium). The calculations are based on relativistic Hartree-Fock wave functions for the atomic bound states and Hartree-Slater wave functions. The results are presented in tabular form such that accurate values of the scattering factors can be obtained by cubic spline interpolation for incident electron energies between 50 and 400 KeV [32].

Mohamed Nasr (2004) calculated the x-ray scattering factor for closed shell atoms for He-like ions (He, Li^+, Be^{2+} and B^{3+}) and Li- like ions (Li, Be^+ and B^{2+}) using Hartree Fock wave function (uncorrelated) published by Clementi and Rotti (1974) and Configuration interaction wave function (correlated) published by Weiss (1961) [33].

1.7 The aim of this work

The research aims are to study and evaluate the x-rays form factor for K-shell and total atom for Li-like ions (Li, Be^+, B^{2+}) and also for Be-like ions (Be, Li^-, B^+) using the uncorrelated wave function by Hartree-Fock of Clementi and Rotti. The importance of the mentioned factor is due to its relation with many important atomic properties.

2.1 The Single Electron Atom

By the early 1900's it had become clear that classical electrodynamics was inadequate to account for the behavior of either the electromagnetic field or of elementary particles. In 1900 Max Planck had shown in his study of black-body radiation that it is necessary to quantize the energy of electromagnetism in order to avoid the "ultra-violet catastrophe", and he introduced the fundamental constant h. In 1905 Einstein made the even more radical proposal that in some respects electromagnetic wave energy propagates as if it consists of small packets (photons) with many of the characteristics of particles, with each photon having an energy E related to the wave frequency ν by $E = h\nu$.

In 1913 Niels Bohr developed a new representation of the hydrogen by combining classical concepts with a few additional postulates that were suggested by the nascent quantum concepts of Planck and Einstein. First, he assumed that the angular momentum of an electron in orbit around the nucleus must be an integer multiple of $\hbar$ (Planck's constant h divided by 2π). It follows that only a certain set of discrete energy levels may occur. Second, he assumed that an electron radiates energy only when it makes a transition from one stable orbit to another of lower energy. If ΔE is the difference in energy levels, then he assumed that the transition resulted in the emission of a photon with this amount of energy, and hence with the frequency $\nu = \Delta E/h$ in accord with Einstein's postulate. Armed with these postulates, Bohr reasoned that an electron of mass m orbiting a proton (of much greater mass) at radius r would satisfy the classical force balance.

A somewhat plausible justification for Bohr's quantization postulate came in 1924 when Louis de Broglie developed the idea that particles of matter on the smallest scale exhibit wave-like properties, analogous to Einstein's suggestion that electro-magnetic waves exhibit particle-like properties. The de Broglie wavelength for the matter wave corresponding to a particle with momentum p is $\lambda = h/p$.

However, despite the plausibility of this approach, Bohr's model of the hydrogen atom, even with de Broglie's justification and with subsequent refinements by Sommerfeld, is now considered obsolete, having been superceded by a more thorough-going wave mechanics developed by Erwin Schrödinger in 1925. (This new theory was subsequently shown to be essentially identical to the "matrix mechanics" developed by Werner Heisenberg in 1924.).

Schrödinger’s wave mechanics postulates that a particle is characterized by a complex-valued wave function $\Psi(x,y,z,t)$ whose squared norm at any point equals the probability density for the particle to be found at that point. (The probability interpretation of Schrödinger’s wave function was first proposed by Max Born.) In addition, Schrödinger postulated that, in a region where there is a potential field $V(x,y,z,t)$, the wave function Ψ of a particle is governed by the equation

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right]+V\Psi=i\hbar\frac{\partial\Psi}{\partial t} \qquad \ldots (2\text{-}1)$$

It's possible to give a plausibility argument for this equation, but here we will just take it as given. If we express the spatial Laplacian (the quantity in the square brackets) in terms of polar coordinates and consider just the radial part, this equation is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Psi(r,t)}{\partial r}\right)\right]+V(r,t)\Psi(r,t)=i\hbar\frac{\partial \Psi(r,t)}{\partial t} \qquad \ldots (2\text{-}2)$$

One expression of the Pauli Exclusion Principle is that (no two electrons in the same atom can be in the same quantum state). This means that no two electrons can have the same set of quantum states of energy, angular momentum magnitude, angular momentum orientation, and orientation of intrinsic spin.

Pauli's Principle is based on the fact that any two given electrons are indistinguishable from one another and thus changing the designations between two or more electrons in different quantum states should have no observable effect. Furthermore, in describing the wave function of an atom, which is the product of the wave functions of the individual electrons. Quantum Physics mandates that the wave function itself (of the atom or electron) is also not observable. On the other hand, the squared magnitude of the atom's wave function is observable, i.e. capable of being experimentally measured. Inasmuch as taking a square root of the squared magnitude of any given wave function will yield a plus (+) or minus (-) sign, the wave function of an atom or elementary particle can either be ***symmetric*** with respect to exchanging the designations of two of its constituent parts (the + sign), or ***anti-symmetric*** (the - sign).

The Pauli Exclusion Principle then specifies the wave functions of electrons, protons and other so-called spin -$\frac{1}{2}$ particles to be anti-symmetric. Thus when two electron designations are switched in the same atom or molecule, the total wave function of the atom or molecule changes sign [1,2].

2.2 The Hartree and Hartree-Fock Approximation

In 1928 Hartree assumed that each electron moves in such an averaged potential arising from the nucleus and the other electrons, and solved Schrödinger's equation for an electron moving in that potential [34]. He chose the wave function of the desired quantum number in that potential and assumed that this wave function is produced from the product of one particle wave function for N-electrons system, i.e.

$$\Psi(1,2,3,...N)=\Phi_1(1)\Phi_2(2)\Phi_3(3)...\Phi_N(N) \qquad ...\ (2\text{-}3)$$

Where $\Phi_i(i)$ depend on the space and spin coordinates of electron i. One major source of difficulty with the total wave function written in the form of the equation (2-3) is the so-called anti-symmetry. This arises from the fact that the Hartree product function incorrectly describes the electron-electron interactions. Electrons have spin ±1/2 entities, and particle with non-integer spins are called fermions, which are characterized by the property of anti-symmetry, where upon when two fermions (electrons) of the same spin are interchanged the wave function changes sign. So the Hartree approximation does not obeys this important property. To avoid this difficulty and, in particular, to let the Hartree product satisfy the Pauli exclusion principle and take into account the indistinguishability of electrons, the total wave function is written as a single Slater determinant [35].

Slater pointed out in the 1920s that choosing the many body wave functions to be of the form [36,37] :

$$\Psi(1,2...N)=\frac{1}{\sqrt{(N!)}}\begin{vmatrix}\Phi_1(1)\Phi_2(1)........\Phi_N(1)\\ \Phi_1(2)\Phi_2(2).......\Phi_N(2)\\ . \quad . \quad .\\ . \quad . \quad .\\ \Phi_1(N)\Phi_2(N)...\Phi_N(N)\end{vmatrix} \qquad \text{... (2-4)}$$

Where, the normalization constant and the component of one particle function $\Phi_i(i)$ is referred to as spin-orbital. Any spin orbital may be written as the product of a space function ϕ and a spin function α or β.

The number in the parentheses denote the particle, and the subscripts (*1,2,...,N*) denote the eigen state. The interchange of any two particles causes the sign of ψ to change, since it involves the interchange of the corresponding two columns, and also when two electrons occupy the same spin orbital, i.e. two columns of the determinate are identical ,the wave function is equal to zero [38].

This observation leads to more familiar expressions of the pauli principle, which states that each orbital may be occupied by only one spin-up and one spin-down electron.

In the Hartree theory, the one-electron orbitals making up the product wave function to minimize the energy were varied, where now the $\Phi's$ in the Slater determinant (2-4) must be varied to get the best possible approximation to the ground-state energy. When this is done, it will be seen that a new set of self-consistent field equations emerge, which differ from Hartree's equations by the appearance of non-classical terms in the self-consistent field.

These are the exchange terms, arising because of the antisymmetry of the wave function (where electrons with parallel spins are present) [39].

Probably the most widely used and most generally successful approach to many-particle quantum mechanics is the independent particle model, which at its beast is represented by the Hartree-Fock (HF) approximation [40].

Physically this approximation amounts to treat the interparticle interactions is only an average fashion, (i.e., each particle is assumed to move in only the field of all the other particles of the system).

Mathematically, the method consists of approximating the state function as an antisymmetrized product of one particle function (spin-orbital).

The idea of the Hartree-Fock self consistent field (SCF) is that each electron is viewed as traveling in a potential. The potential is produced by the interactions between the electron-electron of interest and all the other electrons, and the averaging is over the motion of these other electrons.

Self-consistency enters in that each electron, upon which successive concentration is made, is itself helping to the analogous average field for each other electron, so that orbits must be found that are compatible ultimately for all the electrons simultaneously [41].

Subjecting such a function to the variation principle leads to the well-known SCF equations for the one particle function [40].

The HF 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 electrons 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.

In practice the Hartree-Fock equations are solved numerically by iteration until self-consistent solutions are obtained.

The infinite set of solutions of the HF solutions forms a complete set of one electron functions.

The infinite set of n x n determinantal wave-functions constructed by taking different combinations of n HF solutions form a complete set of n-electron anti-symmetric wave functions.

The exact solutions of Schrödinger's many electron equation may be expressed as linear combinations of these determinantal wave-functions [42]. This approximation with the variation principle leads to the restricted HF equations.

So that the single-electron orbital can then be written as a product of a radial function, a spherical harmonic, and a spin function. This is well-known central-field approximation [1].

The Hartree-Fock wave function also takes some account of correlation between electrons of unlike spin. Of course correlation reduces the energy of the system by keeping electrons a part and the Hartree-Fock method is a better approximation than the Hartree method which completely ignores correlation.

The HF energy is an upper bound to the ground state energy .

The energy difference E(exact) – E(H.F) is called the correlation energy and is a significant measure of the accuracy of the Hartree-Fock method.

The correlation energies for atoms are of the order of a few electron volts.

Roothaan-Hartree-Fock (RHF) or analytic self consistent-field atomic wave function are approximation to conventional Hartree-Fock wave functions in which the radial atomic orbits are expanded as a finite superposition of primitive radial functions.

Since Roothaan's papers and through the early 1970 s, RHF calculations yielded the most accurate atomic HF energies [43,44].

The Hartree-Fock wave function for two or more-electrons is defined as a single Slater determinants as follow [47]:

$$\psi_{HF}\left(1,2,\ldots N\right)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(1)\alpha(1)\ldots\ldots\ldots\ldots\phi_N(1)\beta(1)\\ . \quad . \quad . \quad . \\ . \quad . \quad . \quad . \\ . \quad . \quad . \quad . \\ \phi_1(N)\alpha(N)\ldots.\phi_N(N)\beta(N)\end{vmatrix} \qquad \text{....(2.5)}$$

Where ϕ is the spatial part of the spin-orbital; and α and β refer to the two components of the spin parts (up and down).

The orbitals in turn, are written as an expansion in some set of analytic basis functions [48]

$$\phi_{n\ell}=\sum_i c_n^i X_{n\ell m_\ell}^i \qquad \ldots(2.6)$$

Where: c_n are taken as those which minimize the total energy and the basis function X_{nlm_ℓ} is the standard Slater-type orbitals and is given by:

$$X_{nlm_\ell}(r,\theta,\phi)=R_{nl}(r)Y_{lm_\ell}(\theta,\phi) \qquad \ldots(2.7)$$

And $$R_{nl}(r)=N_{nl}r^{n-1}e^{-\zeta.r} \qquad \ldots(2.8)$$

Where: N_{nl} is the normalization constant and is given as [31]

$$N_{nl}=\frac{(2\zeta)^{n+\frac{1}{2}}}{[(2n)!]^{\frac{1}{2}}} \quad \ldots(2.9)$$

and ζ is the orbital exponents.

3.2 Atomic properties

3.2.1 Two electron density matrix

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 [39, 49, 50]

$$\Gamma_{HF}(x_m,x_n)=\binom{N}{2}\int\Psi(x_1,x_2,x_p,\ldots,x_q)\Psi^*(x_1,x_2,x_p,\ldots,x_q)dx_p\ldots dx_q \quad \ldots(2.10)$$

Where x_n represents the combined space and spin coordinates of electron n, and $dx_p\ldots dx_q$ indicates integration summation over all N-electrons except m and n. The factor $\binom{N}{2}$ ensures that the second order density matrix is normalized to the number of electron pairs within the system:

$$\int\Gamma_{HF}(x_m,x_n)dx_m dx_n=\binom{N}{2}=\frac{N!}{[2!(N-2)!]} \quad \ldots(2.11)$$

Where:

$\binom{N}{2}=6$ for the Be-like ions.

$\binom{N}{2}=3$ for the Li-like ions.

And $\Gamma_{HF}(x_m,x_n)=\sum_{i<j}^{N}\Gamma(x_m,x_n)$ … (2.12)

For Be-like ions

$$\Gamma_{HF} Total = \Gamma_{12} + \Gamma_{13} + \Gamma_{14} + \Gamma_{23} + \Gamma_{24} + \Gamma_{34} \qquad \text{... (2.13)}$$

For Li-like ions

$$\Gamma_{HF} Total = \Gamma_{12} + \Gamma_{13} + \Gamma_{23} \qquad \text{… (2.14)}$$

Then for each Γ_{ij} can be expressed as

$$\Gamma_{ij}(x_m, x_n) = \frac{1}{2}\sum_{i<j}^{N} A_{ij}^{mn}(A_{ij}^{mn})^{*} \qquad \text{… (2.15)}$$

Where

$$A_{ij}^{mn} = \phi_i(m)\phi_j(n) - \phi_j(m)\phi_i(n) \qquad \text{… (2.16)}$$

and ϕ_i is *i*th occupied normalized HF spin-orbital.

By substituting equation (2.16) in equation (2.15) we can written $\Gamma_{ij}(x_m, x_n)$ as follow:

$$\Gamma_{ij}(x_m, x_n) = \frac{1}{2}\sum_{i<j}^{N} [\phi_i(x_m)\phi_j(x_n) - \phi_j(x_m)\phi_i(x_n)]^2 \qquad \text{… (2.17)}$$

the *i* and *j* label occupied spin-orbital and *m*, *n* refer to electron labels [51]. From the above equation the two-electron density in each individual electronic shell in HF can be written as follows:

For **K-shell**:

$$\Gamma'_{12}(K_\alpha k_\beta) = R_{1s}^2(1)R_{1s}^2(2) \qquad \text{… (2.18)}$$

Where prime means integral Γ over spin, (see appendix **A.2)**.

For **KL inter-shell:**

$$\Gamma'_{13}(K_\alpha L_\alpha) = \frac{1}{2}[R_{1s}^2(1)R_{2s}^2(2) + R_{2s}^2(1)R_{1s}^2(2) - 2R_{1s}(1)R_{2s}(1)R_{1s}(2)R_{2s}(2)] = \Gamma'_{24}(K_\beta L_\beta) \qquad \text{... (2.19)}$$

$$\Gamma'_{23}(K_\beta L_\alpha)=\frac{1}{2}[R^2_{1s}(1)R^2_{2s}(2)+R^2_{2s}(1)R^2_{1s}(2)]=\Gamma'_{14}(K_\alpha L_\beta) \qquad \text{... (2.20)}$$

For **L-shell:**

$$\Gamma'_{34}(L_\alpha L_\beta)=R_{2s}{}^2(1)R_{2s}{}^2(2) \qquad \text{... (2.21)}$$

(see appendix **A**.**2**.)

3.2.2 Two-Particle Radial Density Distribution Function

The two-particle radial density distribution *D (r₁, r₂)* in each individual electronic shell is defined by :[26]

$$D(r_1,r_2)=\iint \Gamma'(r_1,r_2)r_1^2r_2^2\,d\Omega_1\Omega_2 \qquad \text{... (2.22)}$$

Where $\Gamma'(r_1,r_2)$ is a spinless function and $D(r_1, r_2)$ tell us how the motion of the two different electrons are correlated as a result of their interactions, $d\Omega_k=\sin\theta_k\,d\theta_k\,d\phi_k$ and $k=1\,or\,2$

Also:

$$\int_0^\infty\int_0^\infty D(r_1,r_2)dr_1dr_2=1 \qquad \text{… (2.23)}$$

That means the two-particle radial density expression $D(r1,r2)\ dr_1dr_2$ is a measure of the probability of finding two electrons such that simultaneously their radial coordinates are in the range r_1 to r_1+dr_1 and r_2 to r_2+dr_2.

Substituting equation (2.18) into equation (2.22), we get the two-particle radial density distribution $D(r_1,r_2)$ for K-shell

$$D(r_1,r_2)=\iint R^2_{1s}(r_1)R^2_{1s}(r_2)r_1^2r_2^2\,d\Omega_1\Omega_2$$

$$=R^2_{1s}(r_1)r_1^2\int Y^*_{1s}(\Omega_1)Y_{1s}(\Omega_1)\sin\theta_1d\theta_1d\phi_1.$$

$$R^2_{1s}(r_2)r_2^2\int Y^*_{1s}(\Omega_2)Y_{1s}(\Omega_2)\sin\theta_2d\theta_2d\phi_2$$

Where:

$$\int Y_{1s}^{*}(\Omega_1)Y_{1s}(\Omega_1)d\Omega_1 = 1$$

$$\int Y_{1s}^{*}(\Omega_2)Y_{1s}(\Omega_2)d\Omega_2 = 1$$

$$D(r_1,r_2) = R_{1s}^{2}(r_1)R_{1s}^{2}(r_2)r_1^{2}r_2^{2} \qquad \text{for K-shell} \qquad \dots (2.24)$$

Following the same procedure above by substituting equation (2-21) into equation (2.22) we get the two particle radial density distribution $D(r_1,r_2)$ for L-shell singlet state, which can be written as:

$$D(r_1,r_2) = R_{2s}^{2}(r_1)R_{2s}^{2}(r_2)r_1^{2}r_2^{2} \qquad \dots (2.25)$$

By substituting equations (2.19) and (2.20) respectively into equation (2.22) we get the two-particle radial density distribution for KL-inter shells Where

$$\int Y_{1s}^{*}(\Omega_1)Y_{2s}(\Omega_1)d\Omega_1 = 1$$

$$\int Y_{2s}^{*}(\Omega_2)Y_{1s}(\Omega_2)d\Omega_2 = 1$$

For $K_\alpha L_\alpha = K_\beta L_\beta$

$$D(r_1,r_2) = [\frac{1}{2}\left(R_{1s}(r_1)R_{2s}(r_2) + R_{1s}(r_2)R_{2s}(r_1)\right)$$
$$- R_{1s}(r_1)R_{2s}(r_2)R_{1s}(r_2)R_{2s}(r_1)]r_1^{2}r_2^{2} \qquad \dots (2.26)$$

For $K_\beta L_\alpha = K_\alpha L_\beta$

$$D(r_1,r_2) = \frac{1}{2}\left[R_{1s}^{2}(1)R_{2s}^{2}(2) + R_{2s}^{2}(1)R_{1s}^{2}(2)\right]r_1^{2}r_2^{2} \qquad \dots (2.27)$$

3.2.3 One Particle Radial Density Distribution Function

The One Particle Radial Density Distribution *D(r1)* is very important for studying the electrons in an atom, which means the probability of finding electrons in each shell. It represents the density distribution of one electron in each shell, and is defined as [26, 52, 53, 49]

$$D(r_1)=\int_0^{\pi}\int_0^{2\pi} r_1^{\,2}\rho(r_1)d\Omega=4\pi\rho(r_1)r_1^{\,2} \qquad \ldots\ (2.28)$$

Where:

$$\rho(r_1)=N\int\Psi(x_1,x_2,x_3,\ldots x_n)\Psi^*(x_1,x_2,x_3,\ldots x_n)d\sigma_1 dx_2 dx_3\ldots dx_n\ldots \qquad \ldots\ (2.29)$$

x_i denotes a combined spatial and spin coordinate, and $\Psi(x_1,x_2,x_3\ldots x_N)$ is normalized wave function.

Evaluation of $D(r1)$ from equation (2.22) by the integration over two-particle density with respect to dr_2 yields,

$$D(r_1)=\int_0^{\infty} D(r_1,r_2)dr_2 \qquad \ldots\ (2.30)$$

The total values of the function D(r1) for different shells in an atom are given by:

For Li-like

$$D_T(r_1)=\frac{1}{3}\left[D_{K\alpha K\beta}(r_1)+D_{K\alpha L\alpha}(r_1)+D_{K\beta L\alpha}(r_1)\right] \qquad \ldots\ (2\text{-}31)$$

For Be-like

$$D_T(r_1)=\frac{1}{6}\left[D_{K\alpha K\beta}(r_1)+D_{K\alpha L\alpha}(r_1)+D_{K\beta L\alpha}(r_1)+D_{K\alpha L\beta}(r_1)+D_{K\beta L\beta}(r_1)+D_{L\alpha L\beta}(r_1)\right]$$

… (2-32)

the evaluation of the one-particle distribution $D(r_1)$ is useful for the determination of (a) the corresponding contribution to the x-ray scattering factor, and (b) one-particle expectation value $\langle r_1^k\rangle$ where $-2\le k\le 2$.

The one-particle density distribution in each individual electronic shell for K-shell can be calculated by substituting equation (2.24) into equation (2.30), i.e.

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

$$=\int_0^\infty R_{1s}^2(r_1)R_{1s}^2(r_2)r_1^2r_2^2dr_2$$

$$=R_{1s}^2(r_1)r_1^2\int_0^\infty R_{1s}^2(r_2)r_2^2dr_2=R_{1s}^2(r_1)r_1^2$$

Where

$$\int_0^\infty R_{1s}^2(r_2)r_2^2dr_2=1$$

$$D(r_1)=R_{1s}^2(r_1)r_1^2 \qquad \dots (2.33)$$

Following the same above procedure by substituting equation (2.25) into equation (2.30) for L-shell one would get,

$$D(r_1)=R_{2s}^2(r_1)r_1^2 \qquad \dots (2.34)$$

The one-particle density distribution for KL-inter shells are equal due to the orthogonality condition between (*1s* and *2s*) orbitals. It can be evaluated by substituting equation (2.26) and (2.27) respectively into equation (2.30)

i.e.

For $K_\alpha L_\alpha$

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

$$D(r_1)=\frac{1}{2}R_{1s}^2(r_1)r_1^2\int_0^\infty R_{2s}^2(r_2)r_2^2dr_2+\frac{1}{2}R_{2s}^2(r_1)r_1^2\int_0^\infty R_{1s}^2(r_2)r_2^2dr_2$$

$$-R_{1s}(r_1)R_{2s}(r_1)r_1^2\int_0^\infty R_{2s}(r_2)R_{1s}(r_2)r_2^2dr_2$$

$$=\frac{1}{2}\left[R_{1s}^2(r_1)+R_{2s}^2(r_1)\right]r_1^2 \qquad \ldots (2.35)$$

Where

$$\int_0^\infty R_{2s}^2(r_2)r_2^2dr_2=1$$

$$\int_0^\infty R_{2s}^2(r_2)R_{1s}^2(r_2)r_2^2dr_2=0$$

The solution of equations (2.33), (2.34) and (2.35) by mathematical analysis are:

For the K-shell is,

$$D(r_1)=\sum_i\sum_j c_ic_jN_iN_je^{-(\zeta_i+\zeta_j)r_1}r_1^{(n_i+n_j)} \qquad \ldots (2.36)$$

For the L-shell is,

$$D(r_1)=\sum_i\sum_j d_id_jN_iN_je^{-(\zeta_i+\zeta_j)r_1}r_1^{(n_i+n_j)} \qquad \ldots (2.37)$$

For the $K_\alpha L_\alpha$ is,

$$D(r_1)=\frac{1}{2}\left(\sum_i\sum_j c_ic_jN_iN_j+\sum_i\sum_j d_id_jN_iN_j\right)e^{-(\zeta_i+\zeta_j)r_1}r_1^{(n_i+n_j)} \qquad \ldots (2.38)$$

Where:

c_i, c_j are the expansion coefficients for *1s* orbital

d_i, d_j are the expansion coefficients for *2s* orbital

N_i, N_j are the normalization constants given by equation (2.9)

3.2.5 Energy expectation values

The energy expectation value related to the potential energy by: [54]

$$< E >= \frac{1}{2} < V > \quad \text{… (2.39)}$$

The potential energy is simply the sum of the electron-nuclear attraction energy and interelectronic repulsion energy, This sum is proportional to the expectation values of $1/r_1$ and $1/r_{12}$ respectively. Therefore we may write:

$$\langle V \rangle = -z\langle \frac{1}{r_1} \rangle + \langle \frac{1}{r_{12}} \rangle \quad \text{…(2.40)}$$

Where z is the atomic number, and [55]:

$$\langle r_1^k \rangle = \int D(r_1) r_1^k dr_1 \quad \text{… (2.41)}$$

$$\langle r_{12}^k \rangle = \int f(r_{12}) r_{12}^k dr_{12} \quad \text{… (2.42)}$$

Here it's assumed that $D(r_1)$ is normalized to the number of electrons and $f(r_{12})$ to the number of electron pairs [54]. The accuracy of results was checked by determining the total energy, it is shown in table [4-19].

3. RESULTS and DISCUSSIONS

This work has been arranged into two parts:

The first is for K-shell, and the second for total atom for Li-like ions (Li atom, Be^+, B^{2+}ions) and Be-like ions (Be atom, Li^-, B^+ ions) which we studied them partitionly as the individually shells and totally. In both parts we have evaluated and plotted the one–particle density distribution function $D(r_1)$, and the atomic form factors $f(s)$.After that a comparison have been made between the individual and corresponding shells in different ions. Each particle distribution function in this work is checked and normalized to unity. The data used in this work are shown in tables (3-1), (3-2), (3-3), (3-4), (3-5) and (3-6).

All these properties have been studied by using Hartree-Fock approximation and by using Mathcad computer program.

3.1 The One-Particle Radial Distribution Function D(r1)

3.1.1 The One-Particle Radial Distribution Functions for K-Shell

The one particle radial distribution function D(r1) is shown as a function of r1 in fig.(3-1) for K-shell of Li and Be like ions. The shapes for distribution functions are approximately the same of the K-shell for Li atom and Li^- ion or Be atom with Be^+ ion and for B^+ ion with B^{++} ion. The curves for D(r1) are starting from zero, it means that there is no probability to finding the electron at the center of the atom, and then increasing to reach the maximum point after that it will decreasing gradually to reach the ending point. The maximum points of D(r1) for (Li, Be^+, B^{++}) are (1.4057, 1.9518, 2.4848) and for (Li^-, Be, B^+) are (1.4063, 1.9448, 2.4848). The different in the maximum points and the ending points with increasing the atomic number Z are due to the attraction force of the nucleus.

The curve will shrink toward the nucleus when the atomic number Z increases, and the peak will increase with decreasing in the broadening curve and the ending point, but the area under these curves are the same due to the normalization condition. The above results are tabulated in table (3-7) for Li-like ions and for Be-like ions.

3.1.2 Total of One-Particle Radial Density Distribution Function

The maximum values of D(r1) increase and the curve shrink toward the nucleus by increasing the atomic number Z due to the increase of attraction force of the nucleus. The density distribution has two peaks for Li-like ions and Be-like ions, one represents the probability of finding the electron in K-shell and the other represents the probability of finding the electron in L-shell. Table (3-8) shows the maximum points for Li-like ions (Li, Be^{+}, B^{++}) and (3-9), (3-10), (3-11) for Be-like ions (Li^{-}, Be, B^{+}). The individual shells and the total of the one particle radial density distribution are shown in figs.(3-2), (3-3), (3-4) for Li-like ions (Li, Be^{+}, B^{++}) and figs.(3-5), (3-6), (3-7) for Be-like ions (Li^{-}, Be, B^{+}), where K-shell have one peak which is greater than the peaks of the other shells, and KL-inter shells are equal in the values for the same element and of the atom and ions of the same atomic number z. For Be-like ions, KL-inter shells and the total of the $D(r_1)$ are equal in the values, and there are two peaks in L-shell, one represents the probability of finding the electron in K-shell and the other represents the probability of finding the electron in L-shell.

Fig.(3-8) shows the comparison of the total one particle radial density distribution for Li-like ions, where the maximum value of $D(r_1)$ increases as the atomic number z increases (i.e. maximum $D(r_1)$ for $B^{++} > Be^{+} >$ Li). Fig.(3-9) shows the comparison of the total one particle radial density distribution for Be-like ions, where the maximum value of $D(r_1)$ increases as the atomic number z increases (i.e. maximum $D(r_1)$ for $B^+ > Be > Li^-$). Fig.(3-10) shows the comparison of the total one particle radial density distribution for Li-like ions and Be-like ions.

3.2 Scattering Form Factor

3.2.1 General Discussions

In studying the scattering form factor for K shell and total for three and four particle system it can be seen that, the form factor starting at the value which equals to the number of electrons at that shell or atom when the scattering angle equals to zero. It means that the total scattering happened, due to the constructive interference of the x-ray wave lengths which is scattered from the electrons, and then gradually decline with increasing the scattering angle until to reach the minimum value. The slownees in the gradual decline and the minimum values are different from one shell to another or from one element to another. The decreasing in the values of scattering form factor when the scattering angle is increasing is due to the partial destructive interference where the path difference of scattered waves from different electrons increases. For the electrons of K-shell where the attraction force toward the nucleus is higher than with the other electrons, the values of the scattering form factor will be greater than of the other shells, and these values increased due to the decreasing in the path difference of the scattered waves. For inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$ of Li like and $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ of Be like, the values of scattering form factor after the maximum point will sharply decrease followed by curvature and then gradually decline, due to charge distribution at the inter shell. Of the electrons of L shell of Be like , where the effective attraction force toward the nucleus is lower than of the K shell, so the electrons are far from the nucleus hence the values of the form factor is lower than of the K shell. The scattering form factor of the intra shells K_α K_β ,L_α L_β are similar in behavior of decreasing with increasing the scattering angle, but they different from the inter shells K_α L_α , K_β L_α , K_α L_β , K_β L_β where the inter shells are similar in behavior of decreasing with increasing angle.

3.2.2 Detailed Discussion

3.2.2.1 Scattering Form Factor for K-shell

For any element of Li-like ions and Be-like ions the scattering form factor starts from maximum value equal to 2, because there are two electrons in the K-shell.

Li atom and Li^- ion: Li atom has three electrons and Li^- ion has four electrons and they have three protons in their nucleus, but they approximately have the same values of scattering form factor due to the same charge distribution, where they decrease gradually after the maximum point with increase the scattering angle, as shown in fig.(3-11) and table (3-12).

Be atom and Be^+ ion: Be atom has four electrons and Be^+ ion has three electrons and they have four protons in their nucleus, but the values of scattering form factor are approximately the same due to the same charge distribution, as shown in fig.(3-11) and table (3-12). The gradual decline is slowly with increasing the scattering angle in comparison with Li atom and Li^- ion.

B^+ and B^{++} ions: B^+ ion has four electrons and B^{++} ion has three electrons and they have five protons in their nucleus, but the values of scattering form factor are approximately the same due to the same charge distribution, as shown in fig.(3-11) and table (3-12).The gradual decline is very slowly with increasing the scattering angle in comparison with the previous elements.

Fig.(3-11) shows the comparison between the atomic form factor for Li-like and Be-like.

3.2.2.2 Total Scattering Form Factor

3.2.2.2.a Total Scattering Form Factor for Li-like Ions

Li atom: table (3-13) and fig.(3-12) show the behavior of atomic form factor for $K_\alpha K_\beta$, K_α L_α , K_β L_α shells and the total of the Li atom. Because the curves KL inter shells undergo sharp dropping in the small values of scattering angle, so the total scattering form factor will have sharp dropping in the small momentum transfers.

Be^+ ion: the values of atomic form factor are presented in table (3-14) and fig.(3-13) for the $K_\alpha K_\beta$, K_α L_α , K_β L_α shells and total of Be^+ ion. The total scattering form factor undergos sharp decline in the small values of momentum transfers due to the sharp dropping in the curves KL inter shells.

B^{++} ion: table (3-15) and fig.(3-14) show the behavior of atomic form factor for $K_\alpha K_\beta$, K_α L_α , K_β L_α shells and the total of the B^+ ion. The total scattering form factor undergos sharp decline in the small values of momentum transfers due to the sharp dropping in the curves KL-inter shells.

Fig.(3-15) shows the comparison between the scattering form factor of Li-like for (K_α L_α , K_β L_α), where the behavior of the curve are approximately the same for the same element (i.e. for the same element $K_\alpha L_\alpha = K_\beta L_\alpha$).

Fig.(3-16) shows the comparison between the total scattering form factor for Li-like ions, where the gradual decline will be slowly with increasing the scattering angle when the atomic number increases (i.e. after maximum point, the values of the total scattering form factor with increasing the scattering angle for $B^{++} > Be^{+} > Li$).

3.2.2.2.b *Total Scattering Form Factor for Be-Like Ions*

The deference between the Li-like ions and Be-like ions is in the number of electrons, in which Li-like ions have three electrons and Be-like ions have four electrons.

Li^- ion: fig.(3-17) and table (3-16) show the behavior of atomic form factor for $K_\alpha K_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$,$L_\alpha L_\beta$ shells and the total of the Li^- ion. Where the values of the inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ are equal because there is no difference between them in distribution of charge.

Fig.(3-18) shows the effect of the ionization on the total atomic form factor for Li atom and Li^- ion. Where each curve, starts from the value which is equal to the number of electrons and then meet at the form factor = 2.35 and s = 0.045, after that they have approximately the same values.

Be atom: fig.(3-19) and table (3-17) show the behavior of atomic form factor for $K_\alpha K_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$,$L_\alpha L_\beta$ shells and the total of the Be atom. Where the values of the inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ are equal because there is no difference between them in distribution of charge.

Fig.(3-20) shows the effect of the ionization on the total atomic form factor for Be atom and Be^+ ion. Where each curve, starts from the value which is equal to the number of electrons and then meet at the form factor = 1.945 and s = 0.117, after that they have approximately the same values.

B^+ ion: fig.(3-21) and table (3-18) show the behavior of atomic form factor for $K_\alpha K_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$,$L_\alpha L_\beta$ shells and the total of the B^+ ion. Where the values of the inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ are equal because there is no difference between them in distribution of charge.

Fig.(3-22) shows the effect of the ionization on the total atomic form factor for B^+ ion and B^{++} ion. Where each curve, starts from the value which is equal to the number of electrons and then meet at the form factor = 1.864 and s = 0.173, after that they have approximately the same values. .

Fig.(3-23) shows the comparison between the scattering form factor of Be-like ions for $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$, where the behavior of the curve are approximately the same for the same element (i.e. for the same element $K_\alpha L_\alpha = K_\beta L_\alpha = K_\alpha L_\beta = K_\beta L_\beta$).

Fig.(3-24) shows the comparison between the scattering form factor for the $L_\alpha L_\beta$ shells for Be-like ions, where the gradual decline will be slowly with increasing the scattering angle when the atomic number increases.

Fig.(3-25) shows the comparison between the total scattering form factor for Be-like ions, where the gradual decline will be slowly with increasing the scattering angle when the atomic number increases (i.e. after maximum point, the values of the total scattering form factor with increasing the scattering angle for $B^+ > Be > Li^-$).

Conclusion and Future Works

4.1 Conclusion

From all these results we can conclude several important points as:

1. The values of the scattering form factor for the K-shell of the atom and ions of the same atomic number are approximately have the same values, and it will be greater than of the other shells.
2. The values of the scattering form factor for inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$ for Li-like ions and $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ for Be-like ions have the same results for the same element, and for atom and ions of the same atomic number Z.
3. After ($\theta = 0$) for Li-like ions or Be-like ions the values of the scattering form factor are increasing with increasing the atomic number Z.
4. The values of the total scattering form factor will be the same for Li atom and Li^- ion after $f(s)= 2.350$ and $s= 0.045$
   Be atom and Be^+ ion after $f(s) = 1.945$ and $s= 0.117$
   B^+ ion and B^{++} ion after $f(s) = 1.864$ and $s=0.173$.
5. The values of the function D(r1) for the K-shell of the atom and ions of the same atomic number are approximately have the same values.
6. The maximum values of the function D(r1) will increase and shrink toward the nucleus when the atomic number Z is increase.
7. The values of the function D(r1) for inter shells $K_\alpha L_\alpha$, $K_\beta L_\alpha$ for Li-like ions and $K_\alpha L_\alpha$, $K_\beta L_\alpha$, $K_\alpha L_\beta$, $K_\beta L_\beta$ for Be-like ions have the same results for the same element ,and for atom and ions of the same atomic number Z.
8. For Li-like ions the values of the total one particle radial density distribution function are one third of the D(r1) for K-shell of the same element.

9. For Be-like ions the values of the total one particle radial density distribution function are one quarter of the D(r1) for K-shell and equal the values of inter shells for the same element.

4.2 Future Works

This work can be extended to include other works, for position and momentum space which are not considered such as:

1. A study of x-ray atomic scattering form factor for K-shell and total atom for three and four electron system using configuration-interaction (CI) wave approximation.
2. A study of incoherent scattering of x-rays $S(s)$ for K-shell and total atom for three and four electron system using HF and CI wave approximations.
3. A study the total differential incoherent scattering cross section $d\sigma_{inc}$ of x-rays using HF and CI approximations.
4. A study the nuclear magnetic shielding constant, connected with x-ray scattering factor for three and four electron system.
5. A study the differential cross section $d\sigma_{el}$ for the elastic scattering of electrons by electrons using HF and CI approximations.

Abstract

The partitioning technique has been used to analyze the three and four electron systems into three-pairs electronic wave functions for Li-like ions (Li, Be^+, B^{++}) and six-pairs electronic wave functions for Be-like ions (Li^-, Be, B^+) by using Hartree-Fock wave functions of Clementi and Rotti.

In this work the atomic scattering factor *f(s)* for K-shell and total atom for three and four electron systems are studied. The physical importance of this factor appears in its relation with the several important atomic properties such as, the coherent scattering intensity, the total scattering intensity, the incoherent scattering function, the coherent scattering cross section, the total incoherent cross section, the nuclear magnetic shielding constant, the differential cross section of electrons scattering from atom and the geometrical structure factor. Also the one particle radial density distribution function *D(r)* has been studied, where the atomic scattering factor *f(s)* is the Fourier transform of the electron density $\rho(r_1)$ and $D(r_1) = 4\pi\rho(r_1)r_1^2$. The accuracy of results was checked by determining the total energy. All results are calculated in atomic units.

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CERTIFICATION

We certify that Mr. Ra'ad Edaan AL-Kenany prepared this thesis under our supervision at Nahrain University in partial fulfillment for the degree of Master of Science in physics.

Signature:

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In view of the available recommendations, I forward this thesis for debate by the examination committee.

Signature:

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(Head of Department)
Date: / / 2006

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Chapter Two: Approximation Methods and Atomic Properties

Chapter Three: Results and Discussions

Chapter Four: Conclusions and Future Works

Examination Committee Certification

We certify that this thesis entitled "***Studying x-ray atomic scattering form factor for K-shell and total atom for three and four electron systems***", is submitted by the student ***Mr. Ra'ad Edaan Al-Kenany*** and as Examination Committee, examined the student in its contents and that in our opinion, it meets the standard of a thesis for the degree of Master of Science in physics.

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Studying x-ray atomic scattering form factor for K-shell and total atom for three and four electron systems

A Thesis
Submitted to the College of Science at Nahrain University
in Partial Fulfillment of the Requirements for the Degree of
Master of Science
in Physics

By

Ra'ad Edaan AL-Kenany
(B.Sc.2003, Nahrain University)

Supervised by

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2006 A.D.

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LIST OF SYMBOLS

Symbol	Meaning
a	Bohr radius
CI	Configuration interaction
c_i	Constant
$d\sigma_{inch}$	Total incoherent scattering cross section
$d\Omega$	Solid – angle element
$f(s)$	Coherent atomic form factor
h	Planck’s constant
$H\,F$	Hartree-Fock
$h\,k\,l$	Miller indices
$I_{c\ell}$	Classical intensity
I_{Th}	Thomson cross section
ℓ	Angular momentum quantum number
m_e	Electron mass
m_ℓ	Magnetic quantum number
$R(r)$	Radial function
$R\,H\,F$	Roothaan-Hartree-Fock
r_0	Classical electron radius
r_{12}	Electron-electron distance
$\mathrm{S}(s)$	Incoherent atomic form function
SCF	Self-consistent field
s	Momentum transfer
$\mathrm{Y}(\Omega)$	Spherical harmonic (angular factor)
Z	Atomic number
$\Gamma(1,2)$	two – electron density matrix
α	Spin up
β	Spin down

ζ	Orbital exponents
λ	Wavelength
ν	Frequency
ξ_{ms}	Spin function
σ_{coh}	Coherent scattering cross section
σ_d	Nuclear magnetic shielding constant
$\sigma_{e\ell}$	Elastic scattering cross section of electron by an atom
ψ	Wave function
ψ^*	Complex wave function
ζ	Orbital exponents
λ	Wavelength
ν	Frequency
ξ_{ms}	Spin function
σ_{coh}	Coherent scattering cross section
σ_d	Nuclear magnetic shielding constant
$\sigma_{e\ell}$	Elastic scattering cross section of electron by an atom
ψ	Wave function
ψ^*	Complex wave function

Chapter one

Introduction
And
Historical Review

Chapter Two

Approximation Methods
And
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Chapter Three

Results and Discussions

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Conclusions and Future works

Appendices

References

الخلاصة

استخدمت تقنية التجزئة لتحليل أنظمة الثلاثة واربعة الكترونات الى ثلاثة ازواج من الدوال الموجية الاكترونية لبعض الايونات المشابهة لذرة الليثيوم وهي $(Li,\ Be^{+},\ B^{++})$، وستة ازواج من الدوال الموجية الاكترونية لبعض الايونات المشابهة لذرة البيريليوم وهي $(Li^{-},\ Be,\ B^{+})$ باستخدام دالة الموجة لهارتري فوك (Hartree-Fock) والمطورة بواسطة كلمنتي وروتي (Clementi and Roetti).

ان هدف البحث هو دراسة عامل الاستطارة الذري للغلاف K والذرة كاملة لانظمة الثلاثة والأربعة الكترونات.

تكمن الاهمية الفيزياوية لعامل الاستطارة الذرية في علاقتة بالعديد من الخواص الذرية المهمة مثل شدة الاستطارة المتشاكهة وشدة الاستطارة الكلية ودالة الاستطارة غير المتشاكهة والمقطع العرضي للاستطارة المتشاكهة والمقطع العرضي الكلي للاستطارة غير المتشاكهة وثابت الحجب المغناطيسي والمقطع العرضي التفاضلي لاستطارة الالكترونات بوساطة الذرات وعامل التركيب الهندسي .

كما تم دراسة دالة توزيع الكثافة القطرية للجسيم الواحد $D(r)$ ، بحيث ان عامل الاستطارة الذري هو تحويل فورير (Fourier transform) لكثافة الالكترون $\rho(r_1)$ وان $D(r_1) = 4\pi\rho(r_1)r_1^2$ ، دقة النَتائِجِ دُقِّقتْ بواسطة حساب الطاقة الكلية. جميع النتائج حسبت باستخدام الوحدات الذرية

جمهورية العراق
وزارة التعليم العالي
والبحث العلمي
جامعة النهرين
كلية العلوم

دراسة عامل الاستطارة الذرية للاشعة السينية للغلاف K والذرة كاملة للأنظمة ذات الثلاث والاربع الكترونات

اطروحة
مقدمة الى كلية العلوم- جامعة النهرين
كجزء من متطلبات نيل درجة
ماجستير علوم
في
الفيزياء

من قبل
رعد عيدان الكناني
(بكالوريوس 2003، جامعة النهرين)

بإشراف
أ. د.خليل هادي البياتي

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