Study of the Properties for Boron Positive Ion in Position Space

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Abstract:

The Hartree-Fock approximation method has been followed to analyze the state of positive boron ion (B^+) into six-pair electronic wave functions, one for *K-shell*, one for *L-shell*, and the rest for enter-shell by means of a new Hartree-Fock wave function.

A theoretical investigation has been carried out on the properties of positive boron ion for intra-shell and inter-shell in position space. The following properties have been investigated in the position space:- (a) the theoretical shape of Compton profile ***J(q)***, (b) the total energy ***E*** and the expectation value of potential energy **<*V*>** and that of kinetic energy**<*T*>,** (c) number of electrons into radius ***r1 [Q(r1)]***.

Due to the importance of the above parameters in investigating the physical and chemical properties of atoms and ions, computer programs in MATHCAD (V.7) have been written to perform the computations concerning the positive boron ion (B^+).

Theory:

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

This approximation with the variation principle leads to the restricted ***HF equations*** as the one- particle radial density distribution $D(r_1)$ [1].

The one-particle radial density distribution $D(r_1)$ 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 [1,2,3,4,5],

$$D(r_1)=\int_0^{\pi}\int_0^{2\pi} r_1^2\rho(r_1)d\Omega=4\pi r_1^2\rho(r_1)\text{......(1)}$$

where:

$$\rho(r_1)=N\int\Psi(X_1,X_2,X_3,..X_N)\psi^*(X_1,X_2,X_3,..,X_N)d\sigma_1 dX_2 dX_3....dX_N\text{ ......(2)}$$

X_i denotes a combined spatial and spin coordinate, and $\psi(X_1,X_2X_3,...X_N)$ is a normalized wave function.

where

$d\Omega_i=\sin\theta_i d\theta_i d\phi_i$ where i = 1 or 2

1- The Compton Profile *J(q)*

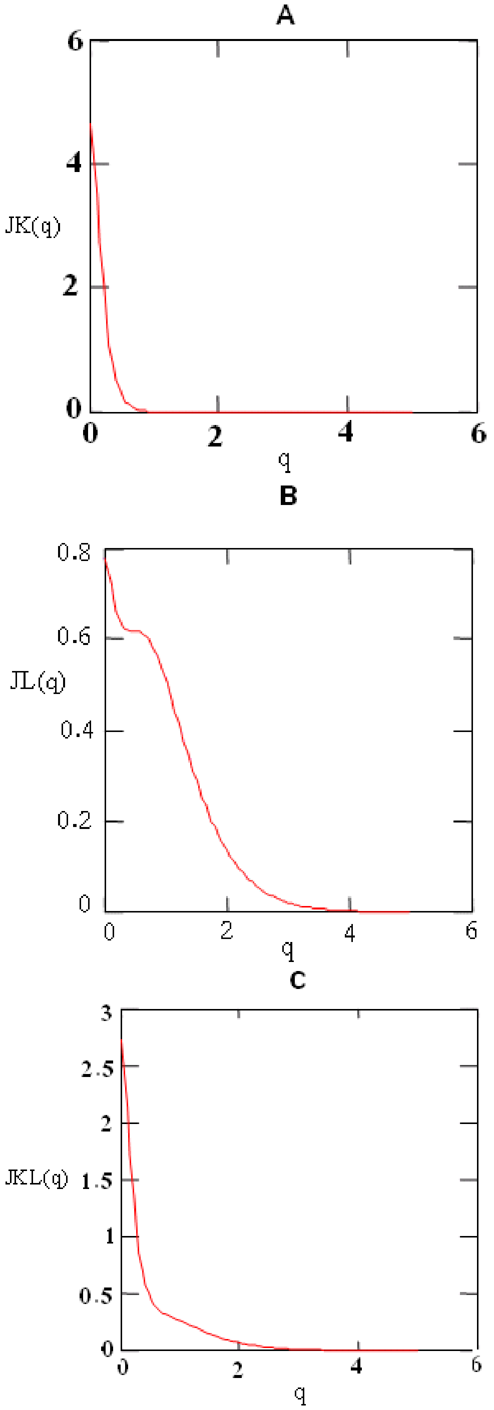
The Compton profile denoted by $J(q)$ is defined as a one-dimensional projection of the electron momentum distribution of all electrons on the choose scattering vector as shown in figure (2). The theoretical shape of the Compton profile for the atom under consideration depends on the value of $D(r_1)$ which is the mean radial distribution function. It should be noted that $D(r_1)dr_1$ is the probability that r_1 has magnitude between r_1 and r_1+dr_1 and its integral is unity by flows equation [6 ,7],

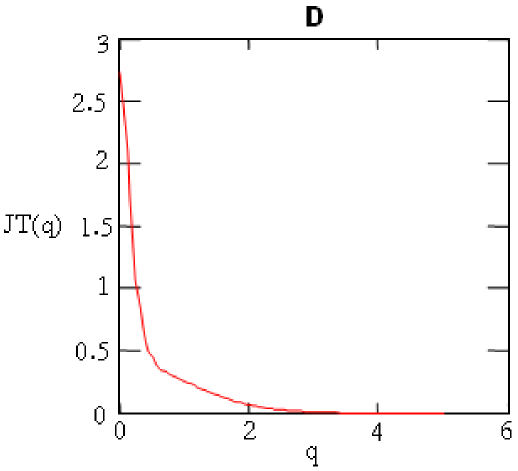
$$\int_0^{\infty} D(r_1)\,dr_1=1$$

$D(r_1)$ may be calculated from the following equation if the momentum wave function $X(r_1)$ is known and there is one electron only,

$$D(r_1)=\int_0^{\infty} X(r_1)X^*(r_1)r_1{}^2dw$$

where dw is an element of solid angle for r_1.





Figure(2): The Compton profile J(q) for B(+ve ion) in {***(A):***K(1s), ***(B):*** L(1s) , ***(C):*** [KL(1s)= KL(3s) and ***(D):***total} shells in position space plotted against q.

The momentum wave function *X(r₁)* is not known directly but may be obtained from the space wave function $\psi(r)$. For one electron, using atomic units, $X(r_1)$ may be defined as [6 , 7],

$$X(r_1) = (2\pi)^{-3/2} \int_0^{\infty} e^{-r.r} \psi(r) d(r)$$

The actual shape of the Compton profile depends on the incident wavelength λ_i and the angle of scattering θ as shown in figure (1). The *J(q)* is given by the following equation as [7],

$$J(q) = \frac{1}{2} \int_q^{\infty} \frac{D(r_1)}{r_1} dr_1 \;......(6)$$

(1/2) is the factor introduced because the normalization condition should be satisfied. From equation (6) the area under the *J(q)* curve is

$$\int_{-\infty}^{+\infty} J(q)dq = 2\int_0^{\infty} J(q) = \int_0^{\infty}\int_q^{\infty} \frac{D(r)dr}{r} dq$$

$$= \int_0^{\infty}\int_0^{p} \frac{D(r)}{r} dq\,dr = \int_0^{\infty} D(r)dr \quad = 1$$

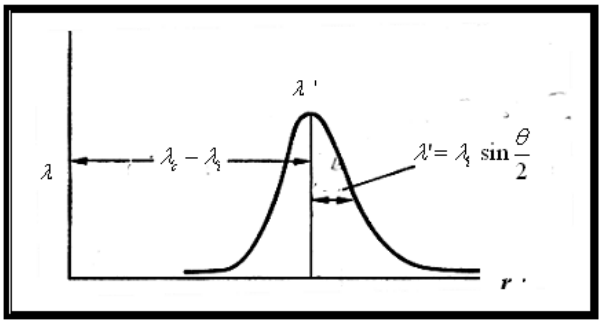


Figure (1):- The Compton profile according to equation (6).

2- The Total Energy *E* and Energy Expectation Values <*V*> and<*T*>

The *Total* energy of B^+ ion can be determined for an N–electron atomic wave function by the following **Benesch** equation [8,9],

$$E_{Total} = -\frac{1}{2} \int_0^{\infty} r_1^2 D(r_1) dr_1 \;......(7)$$

Therefore the kinetic energy *T* and the potential energy *V* can be determined from the following equation [10,11],

$$E_{Total} = -< T > = \frac{1}{2} < V > ......(8)$$

In position space, the potential energy is simply the sum of the electron–nuclear attraction energy $< r_1^{-1} >$ and the interelectronic expectation energy $< r_{12}^{-1} >$. Therefore the expectation value of the potential energy can be written in a from as follows,

$$< V > = -z. < r_1^{-1} > + < r_{12}^{-1} > ......(9)$$

Where *z* is the number of electrons which is equal to 4 in B^+ ion, therefore the magnitudes of total energy, the expectation values of potential energy and kinetic energy can be obtained as in table [1]

***E* Total energy**	**$\langle V \rangle$ *Potential energy expectation value***	**$\langle T \rangle$ *Kinetic energy expectation value***
-0.071	*-0.143*	*0.071*
-1.913	*-3.826*	*1.913*
-0.992	*-1.984*	*0.992*
-0.992	*-1.984*	*0.992*
-0.992	*-1.984*	*0.992*

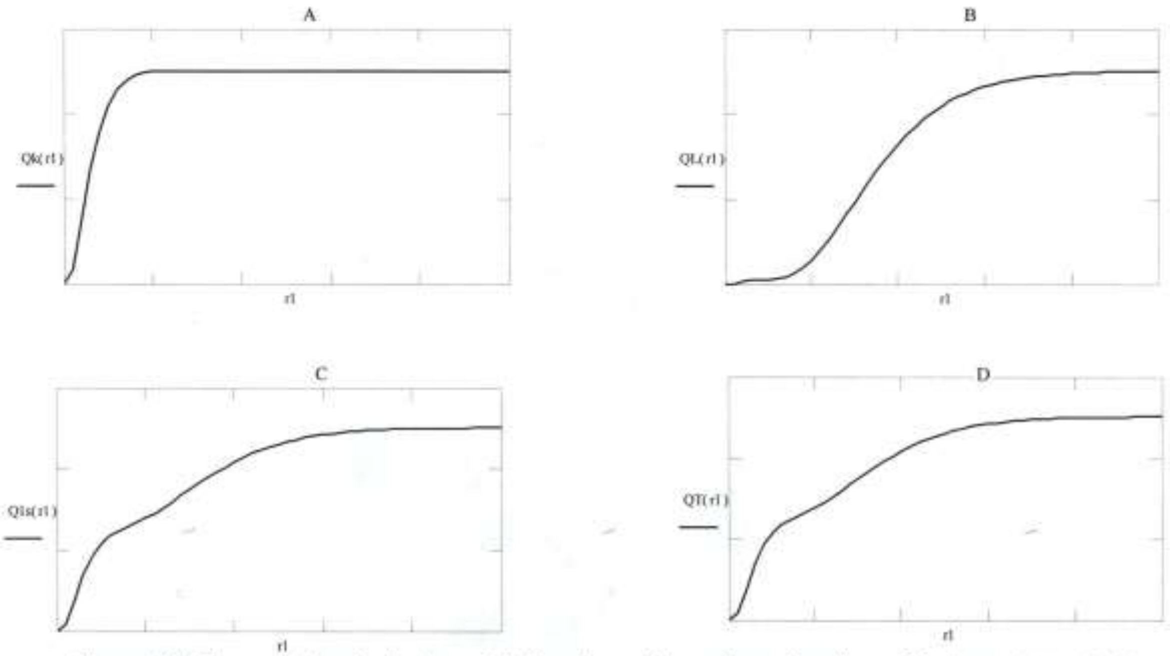
Table (1):- The magnitudes of total energy, the expectation values of potential energy and the expectation values of kinetic energy for B (+ ion) in position space.

3-The Number of electrons enclosed within sphere of radius *r1 Q(r1):-*

The number of electronics enclosed in sphere of radius r1 centered on the nucleus ***Q(r1)*** as shown in figure(3), represent the electron-static potential at the nucleus due to the electron cloud [12,13],

$$Q(r_1) = \int_0^{r_1} 4\pi r_1^2 \rho(r_1) dr_1 ......(10)$$

Some moments of radial electron density in closed- shell atoms and their atomic scattering factors.



Figure(3): The numberof electrons **Q(r1)**enclosed in aspher of radius ***r1*** for intra, inter shells and total for *B(+veion)* in each individual electronic shells plotted against ***r1*** in position space when (A):K(1s),(B):L(1s),(C):KL(1s=3s) and (D):Total.

Results And Discussion:

1-1 The Compton profile *J (q)* :-

The Compton profile *J(q)* for B^+ ion in intra-*shell* is shown in figure (2). The maximum value of *J (q)* for *K-shell* and *L-shell* is found at *q=0;* they are the maximum Compton scattering of x-ray when sin θ=1 (i.e., at θ=90) as shown in figures (2-A) and (2-B). It can be seen from these figures that the *J (q)* distribution changes abruptly as it departs away from the nucleus. The *J(q)* distribution for *K-shell* is steeper than that for the *L-shell* because it is related to the spherically averaged momentum density as given in equation (6). The range of the value of *q* is very small for *K-shell* compared with that for the *L-shell* as shown in figure (2) and it have two peaks where it has one peak in *K-shell*. The maximum value of *J(q)* for *K-shell* is greater than that for the *L-shell*.

In the inter-shell, The maximum of *J(q)* for $KL(\,^1s)$-and $KL(\,^3s)$ states is at *q*=0 as shown in figure(2-C) and(2-D) . The curve in inter-*shell* is steeper than that of the intra-*shell*. The *J(q)* in $KL(^1s)$, $KL(^3s)$ and *Total* state has the same form, because the one particle radial density distribution $D(r_1)$ has the same value in $KL(\,^1s)$, $KL(\,^3s)$ and *Total* state.

2-2 The Total energy *E* and expectation value < *V* > and < *T* > :-

The *Total* energy *E*, the potential energy expectation value < *V* >, and the kinetic energy expectation value < *T* >, given in table [1] have been calculated with the aid of equation (3) and (4) for intra-and inter-shells and the *Total*. The *Total* energy *E* and < *T* > are numerically equal but have opposite signs. Furthermore, < *V* > is twice the value of *E*.

3-3The number of electrons Q(r1)enclosed in sphere r1:-

The number of electrons enclosed in sphere of radius r1 centered on the nucleus *Q(r1)* for B^+ ion in intra-*shell* is shown in figure (3) and it has the opposite behavior to that in *J(q)* . The minimum value of *Q(r1)* for *K-shell* and *L-shell* is found at *r1=0,* as shown in figures (3-A) and (3-B). It can be seen from these figures that the *Q(r1)* distribution changes abruptly as it departs towards the nucleus. The *Q(r1)* distribution for *K-shell* is very high value where magnitude of r1 increase but in *L-shell* has graduated high as shown in figure (3-A) and (3-B).

In the inter-shell, The maximum of *Q(r1)* for $KL(\,^1s)$-and $KL(\,^3s)$ states is at *r1*=0 as shown in figure(3-C) and(3-D) . The *Q(r1)* in $KL(\,^1s)$, $KL(\,^3s)$ and *Total* state has the same form, because the one particle radial density distribution $D(r_1)$ has the same value in $KL(\,^1s)$, $KL(\,^3s)$ and *Total* state.

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دراسة خصائص الايون الموجب للبورون في فضاء المكان

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الملخص:

إن طريقة التقريب لدالة الموجة الجديدة لهارتري فوك قد أتبع لتحليل حالة أيون البورون الموجب (B^+) لستة أزواج دوال موجية إلكترونية، واحدة للغلاف K ، وواحدة للغلاف L والبقية للقشرة الوسطية(KL^3s,KL^1s). إذ جرت دراسة نظرية لخصائص أيون البورون الموجب للقشرة الواحدة وللقشرة الوسطية في فضاء المكان.

إن الخواص التي تمت دراستها في فضاء المكان هي (أ) هيئة كومبتن، (ب) الطاقة الكلية والقيم المتوقعة للطاقة الكامنة والطاقة الحركية، (ج)عدد الألكترونات المتواجدة في ذرة نصف قطرها r1.

ولأهمية المعاملات المذكورة أعلاه في دراسة الخواص الفيزياوية والكيماوية للذرات فقد وضعت برامج حاسوبية في ال{MathCAD (V.7)} لإجراء الحسابات الخاصة بأيون البورون الموجب.