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Review

Momentum evaluations of the electron-nuclear shielding constant for many-electron systems

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Hartree Fock (HF) wave function in momentum space Nuclear magnatic shelding constant calculation are determind for the ground states of the folowing member of|Li-isoelectric series :Li,Be^{+}, $B^{+2,}$ C^{+3} , N^{+4} ,O^{+5} ,Fe^{+6} ,and Ne^{+7} .For each speices, the density distribution function *D(p₁)* the electron density at nucleus, moments of $<p^n_i>$ for n=-2,-1 to 2, and diamagnetic suscbtability are reported using MathCad program.

Keywords : Mumentum, Electron, Nuclear, Electron Systems

INTRODUCTION

Auseful working discription of the electronic structure in atoms or ions is provid by the independent particle model.The analysis is applied here to the ground stste of Li. By partitioning the second order density as proposed by (Banyard and Youngman, 1987) (Valley and Alley, 2002).

The prime example of this search is HF treatment. HF theory is the use of asingle-determinant wave function Ψ which is formed from a set of occupied spin orbitals x_1, x_2 , x_3 , ……..,x_n (Thakkarjit and Vedene, 1978)

$$\Psi = A\det\{x_1, x_2, x_3, ...x_n\} \quad (1)$$

Where n is the number of electrons. A is a normalization constsnt and the diagonal element product of determinent to saatisfied explicitiy in eq.1.

X_n is the doublet spin eigenfunction and the functional form employed is

$$x = \alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3) \quad (2)$$

THEORY

Ageneral analysis of the ^{2}S-state of the Li I isoelectronic series in the same spirit as king hasrecently been carred out (Banyard et al., 1988) .The radial electronic density distribution functions $D_0(p)$ is evaluated for N-electron systems using (Banyard et al., 1988):

$$D_o(p) = \int_0^{\pi}\int_0^{2\pi} p^2 \rho(p)\, d\Omega \quad (3)$$

$$\rho(p) = N\int \Psi^*(x1, x2, ...xn) X \Psi(x1, x2, ...xn) ds dx2 dx3 ....dxn \quad (4)$$

Wher standerd notation $d\Omega = \sin\theta d\theta d\phi$
And x_i denoted a combined spatial and spin coordinate and
Is normalized wave function and in present work N=3.Ψ(x1,x2,….xn)

Table I. Radial Density Distribution Fuunction , Electron Density At The Nucleus:

Species	shell	D_0(r)x.	Location $\rho(0)$	$p1$
Li	KαKβ	0.544	0.127	0.3
Be+	KβKα	0.324	0.083	0.5
B^{+2}	KαKα	0.228	0.015	0.6
C^{+3}	KαKα	0.182	2.175-03	0.9
N^{+4}	KαKα	0.150	5.545-03	1.1
O^{+5}	KαKα	0.128	1.780-04	1.3
F^{+6}	KαKα	0.111	7.595-05	1.4
Ne^{+7}	KαKα	0.099	3.710-05	1.5

Table II. Expectation Values For The Intra Shell(K-Shell)For Li –Isoelectronic Series :

Species	n				
+2	-2	-1	0	+1	
Li	0.76422	0.657109	0.999999	2.246038	7.223937
Be+	0.396380	0.474361	0.999999	3.092023	13.57525
B^{+2}	0.241883	0.371072	1.000000	3.938945	21.92341
C^{+3}	0.162729	0.304664	1.000000	4.786131	32.26986
N^{+4}	0.11683	0.258356	0.999999	5.63409	44.61596
O^{+5}	0.087981	0.224287	0.999999	6.482112	58.96018
F^{+6}	0.06859	0.198129	0.999999	7.330403	75.30776
Ne^{+7}	0.054269	0.177433	0.999998	8.17861	93.653734

The wave function employed in this study are Hartree-Fock type (Landau and Lishitz, 1974).

$$\Psi(x_1, x_2, x_3) = A\,\phi_N(x_1, x_2, x_3)$$

$$\Psi(x_1, x_2, x_3) = A\sum_{\mu}^{N} C_\mu \phi_\mu \qquad (6)$$

Where A is the antisymmetrizer , are the variation ally determined expansion coefficients ,N is the number of basis function .

COMPACT FORMULA OF $D_0(p)$

The one particle radial Expectation values can be obtain [5]

$$\langle p_i^n \rangle = \sum_{-1}^{3} \langle \Psi | p_1^n | \Psi \rangle$$

$$\langle p_i^n \rangle = \int_0^{(5\infty)} D_o(p)\, p^n\, dp$$

The required formula of the one particle radial density distribution function is:

$$D_o(p) = C_\mu C_N \left[\frac{(2\xi_\mu)^{n_\mu = 0.5}}{\sqrt{(2n_\mu)}} \frac{(2\xi_\mu)^{n_N + 0.5}}{\sqrt{(2n_N)}} \right] p^{n\mu - 1}\, p^{nN - 1}\, e^{-(\xi\mu + \xi N)p}$$

The one particle expectation values is:

Table Iii: Expectation Values For The Intra Shell(L-Shell) For Li –Isoelectronic Series :

Species	**n**				
	-2	**-1**	**0**	**+1**	**+2**
Li	5.046617	3.872695	0.999999	0.413496	0..417639
Be+	8.224346	2.205598	0.999999	0.766091	1.404733
B^{+2}	4.141884	2..371072	1.000000	1.112376	2.906504
C^{+3}	2.501313	1.207308	0.99989	1.456210	4.913969
N^{+4}	1.674565	0.985904	1.000000	1.798962	7.424515
O^{+5}	1.200417	0.833497	0.999999	2.231450	10.435781
F^{+6}	0.903436	0.722215	0.999999	2.481965	13.949432
Ne^{+7}	0.721308	0.654871	0.999998	2.862836	18.043641

Table VI : Expectation Values For The Inter Shell(Kl-Shell) For Li –Isoelectronic Series :

Species	**n**				
	-2	**-1**	**0**	**+1**	**+2**
Li	12.905423	2.264902	1.000000	1.329767	3.820788
Be+	4.310366	1.339979	0.999999	1.929057	7.489979
B^{+2}	2.191884	0.964646	0.999999	2.525660	12.414957
C^{+3}	1.332021	0.755976	1.000000	3.121264	18.59191
N^{+4}	0.895698	0.622130	0.999999	3.716531	26.02024
O^{+5}	0.644199	0.528892	0.999999	4.311427	34.69798
F^{+6}	0.486013	0.460172	1.000000	4.966185	44.628599
Ne^{+7}	0.388139	0.4161521	0.999999	5.520758	55.848681

$$\langle p_i^n \rangle = \langle R_{1s} \left| p^{n+2} \right| R_{1s} \rangle \quad (10)$$

$$\langle p_i^n \rangle = \langle \sum_{\mu} S_{\mu\ell} C_{\mu\ell} \left| p^{n+1} \right| \sum_{N} S_{N\ell} C_{N\ell n} \rangle \quad (11)$$

$$\langle p^n \rangle = \langle S_{1\ell} C_{1\ell n} \left| p^{n+2} \right| S_{1\ell'} C_{1\ell' n'} \rangle \quad (12)$$

$$\langle p_i^n \rangle = \langle \sum_{\mu} N_{\mu\ell}\, p^{(n\mu\ell-1)}\, e^{(-\xi\mu\ell)p1} C_{\mu\ell n} \left| p^{n+2} \right| \sum_{N} N_{N\ell}\, p^{(nN\ell-1)}\, e^{(-\xi\mu\ell)p1} C_{N\ell n} \rangle$$

Where

$S_{\mu\ell}$ and $S_{N\ell}$ takenas Slatertypeorbitals

$S_{\mu\ell}$ and $S_{N\ell}$ is the normalization factor

$n_{\mu\ell}$ and $n_{N\ell}$ is the principle quantum number

$\xi_{\mu\ell}$ and $\xi_{N\ell}$ is the orbital exponent

ℓ is a azmeithal quantum number

$$N_{\mu\ell} = \frac{(2\xi_{\mu\ell})^{n_{\mu\ell}+0.5}}{\sqrt{(2n_{\mu\ell})}} \quad and \quad N_{N\ell} = \frac{(2\xi_{N\ell})^{n_{N\ell}+0.5}}{\sqrt{(2n_{N\ell})}} \quad (14)$$

$$\langle p^n \rangle = \langle S_{1\ell} C_{1\ell n} \left| p^{n+2} \right| S_{1\ell'} C_{1\ell' n'} \rangle \quad (15)$$

$$\langle p^n \rangle = \langle S_{1\ell} C_{1\ell n} \left| p^{n+2} \right| S_{1\ell'} C_{1\ell' n'} \rangle \langle S_{2\ell} C_{2\ell n} \left| p^{n+2} \right| S_{2\ell'} C_{2\ell' n'} \rangle$$

$$(13)\ \langle S_{3\ell} C_{3\ell n} \left| p^{n+2} \right| S_{3\ell'} C_{3\ell' n'} \rangle \quad (16)$$

$$\rho(0) = \left\{ \frac{D_o(p)}{4\pi p^2} \right\}_{p \to 0} \quad (17)$$

$$\rho(0) = \langle \delta(p_i) \rangle \quad (18)$$

Table IV : Nuclear Magnetic Sheilding Constant And Diamagnetic Suscubtability For Li –Isoelectronic Series :

Species	shell	σ	χ
Li	KαKβ	1.166-05	-6.411-05
	LαLβ	6.874-05	-3.707-06
	KαLβ= KβLα	4.021-05	-3.391-05
Be+	KαKβ	8.420-06	-1.205-04
	LαLβ	3.915-05	-1.247-05
	KαLβ= KβLα	2.379-05	-6.648-04
B^+	KαKβ	6.586-06	-1.946-04
	LαLβ	2.766-05	-2.580-05
	KαLβ= KβLα	1.712-01	-1.102-04
C^{+3}	KαKβ	5.408-06	-2.864-04
	LαLβ	2.143-05	-4.361-05
	KαLβ= KβLα	1.342-05	-1.650-04
N^{+4}	KαKβ	4.586-06	-3.960 -04
	LαLβ	1.750-05	-6.589-05
	KαLβ= KβLα	1.104-05	-2.309-04
O^{+5}	KαKβ	3.981-06	-5.233-04
	LαLβ	1.479-05	-9.262-05
	KαLβ= KβLα	9.388-6	-3.081-04
F^{+6}	KαKβ	23.51-06	-6.684-04
	LαLβ	1.282-05	-8.238-05
	KαLβ= KβLα	8.168-05	-3.961-04
Ne^{+7}	KαKβ	3.151-06	-8.312-04
	LαLβ	1.162-05	-1.601-05
	KαLβ= KβLα	7.387-05	-4.957-04

DISCUSSIION

A- CALCULATION OF ELECTRON DENSITY AT THE NUCLUES $\rho(0)$

From equation (3), the electron density at the nucleus can be evaluated using (King, 1988):

$$\rho(0) = \left\{ \frac{D_0(p)}{4\pi\, p^2} \right\}_{p \to 0} \quad (17)$$

Because of the simple analytic form obtained for one particle radial density in the integral (eq.8)is trivial evaluate the electron density at the nucleus

$$\rho(0) = <\delta(p_i)> \quad (18)$$

In table I, the electron density at the nucleus $\rho(0)$ depends on the one particle radial density distribution $D(p_1)$ and the results of $D(p_1)$ is decreases as atomic number increases the electron nuclear cusp condition are infairly reasonable agreement, which improves with increasing charge.

B- ONE PARTICLE RADIAL DENSITY DISTRIBUTION FUNCTION $<p_i^n>$:

From the radial expectation values given in tables II,III,VI respectively we notice that the effect of electron correlation is to reduce $<p_i^n>$ for each n ,indicating that the magnitude of the on the one particle radial density distribution has been decreases for all p_i . For each Z the one particle radial expectation values decreases when n goes from -1 to -2 ,and increases when n goes from 1 to 2 , that means the expectation value weight different regions of space (i.e the probability of finding the electrons in the region near the nucleus or farther away from it).when n=1,and 2, the one particle expectation value$<p_i^n>$ increases by increasing the atomic number Z, this is due to the Coulomb attraction force of the nucleus to the charge which leads to increase the probability of finding the electron near the nucleus .For negative values of *n* , the expectation values decreases by increasing the atomic number Z due to the weakly Coulomb attraction force between the nucleus and the electrons in the outer shells.

Correlation also produces a shift in the towards higher momentum since we observe an increase in both $<p>$ and $<p_i^2>$. The normalized condition can be can be obtained from the calculation of one particle expectation value $<p_1^n>$ at ($n=0$) and this state may be applied for all shells. By examining all expectation tables for the Li-atom, Li-like ions we found that the value of *LαLβ* is greater than those for *KαKβ* because it is the outer most shell (i.e in momentum view the inner most shell *LαLβ* to the outer most shell *KαKβ*), the two state decreases when then atom number (Z) increase too.

C-NUCLER MAGNETIC SHEILDING CONSTANT σ AND DIAMAGNETIC SUSCUBTABILITY χ

Table IV show the results of the nuclear magnetic shielding constant σ *KαKβ* is greater than that found for *LαLβ* due to the diamagnetic shielding factor ( ) for *LαLβ*, and this is not found for *KαKβ* because the charge for the two electron in the *KαKβ* will reduce the nucleus shielding to the *LαLβ*. As Z increases the nuclear magnetic shielding constant σ decreases in momentum conclusions.

The diamagnetic susceptibility for Li-isoelectronic series for *KαKβ* is less than that for *LαLβ*, *KβLα* , *KαLβ* because the diamagnetic susceptibility depends on the radius of 1s and 2s respectively.

Also this can be confirmed by comparing the moment $<p_1^n>$ at n = 2 From comparison between χ for Li-atom and χ for Li-like ions, it is observed that the diamagnetic susceptibility decreases as Z (atomic number) increases, because the radius of 1s and 2s for positive ions is smaller than that for Li-atom due to the attraction force between the electron and the proton. This conclude agree with the relation between σ and $<p_1^{-1}>$ from equation (8)

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