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Evaluation of Diamagnetic Susceptibility for B^+ ion

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ABSTRACT

Configuration Interaction wave functions determined by Weiss in 1961[1]for intra-and inter shell correlation effects of two electron systems have been examined in position space. The required partitioning of the correlated second order density matrix was arrived here, up to and including the pair-correlation effects. Diamagnetic susceptibility was determined within individual electronic shells for B^+*(four electron systems)compared with Be system in their ground state. All results of diamagnetic suscbtability are reported using MathCad program.*

Keywords: Theoretical Physics, Boron atom.

INTRODUCTION

Diamagnetism is the phenomenon of a magnetic field .In other words, a diamagnetic material has a negative magnetic susceptibility .The diamagnetic susceptibilities are very small in magnitude compared to paramagnetic materials, and negligible compared to ferromagnetic materials. The universally accepted explanation of diamagnetism is the precession of the magnetic moment created by the orbital motion of electrons. Diamagnetism is conceptually simple and can be quantitatively explained to a high degree of accuracy. To a close approximation the diamagnetic susceptibility of a compound is the sum of the susceptibility of its components. But the components of a molecule as far as its diamagnetic susceptibility is concerned is probably its electron bonds rather than its atoms and their electrons. Thus the contribution of an atom to a compound depends upon the other constituents of the compound. The simple notion that if two entities, atoms or ions, have the same number of electrons then they will have the same electronic structure and hence the same diamagnetism is not always valid. Sometimes the difference of one unit of charge in the nucleus will alter the energy levels and consequently change the minimum energy configuration. [2].

MATERIALS AND METHODS

Theory: In the quantum theory of the electronic structure of matter, the two-electron systems provide a valuable bridge between the comparatively simple one-electron systems and systems containing many electrons. The structure of an electronic system within a given nuclear framework depends not only on the balance between the kinetic energy of the electrons and their attraction to the nuclei, but also on the mutual electronic repulsion. The latter effect cannot be treated within the conventional "one-electron approximation" for accurate solution of the many-electron Schrödinger equation. Therefore, other methods are in vogue[3], and the results for two-electron systems are then also of guiding importance in treating systems containing many electrons[4]. The correlated wave functions were formulated either by means of configurations interaction (CI) treatment, or by the inclusion of explicit correlation factors. The CI wave function was those of Weiss, and the r_{12} functions were those of Green et al. Both types were first investigated by Hyllera as in his pioneering work on the helium atom. Hyllera has found that the series of configurations converged rather slowly and that a much quicker convergence could be obtained by introducing r_{12} explicitly in the solution. The method of"configuration interaction"has the great advantage that it may be directly generalized to many-electron systems. [5]

The One Particle Radial Expectation Values: The moment $<r_1^n>$ can be calculated from

$$<r_1^n>_{ij} = \int D_{ij}(r_1)\, r_1^n dr_1 \qquad (1)$$

Where $D_{ij}(r_1)$ is the one particle distribution function, and r_1 = the distance from the nucleus to the electron "1" in unit of Bohr radius. $-2 \le n \le 2$, the case n = -1 one can calculate the electron nuclear potential energy and nuclear magnetic shielding constant from the moment $<r_1^{-1}>$, n = +2 is required to evaluate the diamagnetic susceptibility, n = 0 the result of $<r_1^n>$ must be equal to one (normalization condition), n = 1 required to the position, and n = 2 gives the angular momentum [6].

Diamagnetic Susceptibility χ : The diamagnetic susceptibility is defined by [7]

$$\chi = -\frac{1}{6}\alpha^2 <\psi\left|\sum_{i=1}^{n}(r_i^2)\right|\psi> \qquad (2)$$

Where α is the fine structure constant and it is equal to (7.297353 x 10^{-3} au).And the molar diamagnetic susceptibility χ_m (in the standard employed units of $cm^3\ mol^{-1}$) is given by:

$$\chi_m = -\frac{1}{6} N_A \alpha^2 a_\circ^3 <\psi\left|\sum_{i=1}^{n}(r_i^2)\right|\psi> \qquad (3)$$

Where N_A is Avogadro's number, a_o is the Bohr radius. Using the values: $N_A = 6.221367 \times 10^{23}\ mol^{-1}$ and $a_\circ = 0.529177249 \times 10^{-8} cm$

Leads to χ in unit of $cm^3\ mol^{-1}$ as [8]:

$$\chi_m = -0.7920153(4) \times 10^{-6} <\psi\left|\sum_{i=1}^{n}(r_i^2)\right|\psi> \qquad (4)$$

If χ_m is positive the material is called paramagnetic, and if χ_m is negative the material is called diamagnetic [9].
Thus
$|\chi_m| << 1$ (for paramagnetic and diamagnetic) .From the diamagnetic susceptibility we can be calculating the cross section for elastic scattering as [10]:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\theta=0} = \frac{\gamma^2}{9} <r_i^2>^2 \qquad (5)$$

Where γ^2 is the factor $[1-(v^2/c^2)]^{-1}$, v is the electron velocity, and c is the speed of light.

RESULTS AND DISCUSSION

The normalized condition can be obtained from the calculation of one particle expectation value $<r_1^n>$ at (n=0) and this state may be applied for all shells (figure 1). A perusal of table 1 shows , the one particle expectation values for each individual electronic shells for B^+ , and Be-atom , For B^+(positive Boron ion) is greater than those for the Be atom at n = -ve, whereas for n= +ve the result for Be atom is greater than those for B^+. This is as a result of the K-shell shrinkage increases the attraction force between electron and the nucleus .The values of the one particle expectation values increases when n goes from -1 to -2 , and decreases when n goes from 1 to 2, as a result of electron distance related to the nucleus. Also the result of KL (^1S) is similar in value to KL (^3S) because there is no cross term, from the two particle distribution function and these values are equal to [K(^1S) + L(^1S)]

$$D_{ij}(r_1,r_2)=\frac{1}{2}r_1^2r_2^2\left[R_{1S(1)}^2R_{2S(2)}^2+R_{2S(1)}^2R_{1S(2)}^2\right]$$
$$+r_1^2r_2^2\left[R_{1S(1)}R_{2S(1)}R_{2S(2)}R_{1S(2)}\right]$$

$$\text{----------------------------}$$

Cross Term

Referring to table (1) we see that the standard deviation Δr_1 for K- shell is smaller than that found in L-shell since we have Δr_1 determine the diffuse of the one particle radial density distribution $D(r_1)$ and we have the location of r_1 for K- shell is smaller than that for Be atom and for all of them the value of K- shell is smaller than that for L- shell so we found that the standard deviation Δr_1 for K- shell is smaller than that found in L – shell. Reference [10] shows good agreements with the B^+ results in both tables.

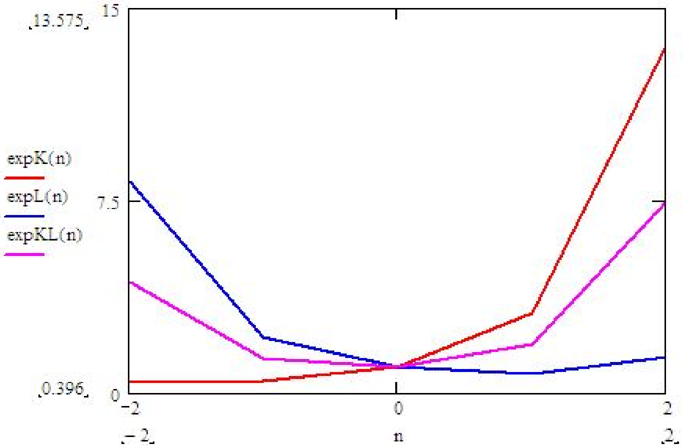

Figure 1. The one particle radial expectation values of K-, L- , and KL-shells for B^+ ion

For the ^2S ground states of atomic system studied in this work, the values of χ are tabulated in table (II), which is illustrate that the diamagnetic susceptibility for B+ve for K (^1S) is less than that for L (^1S), KL(^1S), KL(^3S), and total because the diamagnetic susceptibility depends on the radius of 1s and 2s respectively. Also this can be confirmed by comparing the moment $<r_1^n>$ at n = 2 (see eq. (1)). From comparison between χ for B+ve and χ for Be-atom , it is observed that the diamagnetic susceptibility decreases as Z (atomic number) increases, because the radius of 1S and 2S for B+ve ion is smaller than that for Be atom due to the attraction force between the electron and the proton .The same discussion apply for the diamagnetic susceptibility for the inter- shells KL (^1S) and KL (^3S) (see eq. (2)).

Table 1 .Expectation Values For The Inter Shell(Kl-Shell)For Li- Isoelectronic Series

Species				**n**		
SHELL	ATOM	**-2**	**-1**	**0**	**+1**	**+2**
K	B^+	44.607	4.679	1.000	0.325	0.142
	Be	27.753	3.681	1.000	0.450	0.233
L	B^+	2.415	0.780	1.000	1.798	3.825
	Be	1.055	0.522	1.000	2.649	8.426
KL	B^+	23.516	12.729	1.000	1.061	1.984
	Be	14.404	12.102	1.000	1.532	4.312
Total						
	B^+	23.516	12.729	1.000	1.061	1.984
	Ref[10]	23.510	2.725	1.000	1.060	1.982
	Be	14.404	2.102	1.000	1.532	4.312

Table 2. Diamagnetic And Molar Diamagnetic Susceptibilityχ , χ_M In Units Of (Cm^3/Mol) For B+Ve Ion And Be Atom For Each Individual Shell(Datat For Be Was Taken From Ref. [10] .

Atom	**shell**	**χ-**	**χ_m (cm^3/mol)**
KαKβ	**B^+**	1.2663-06	1.8833-08
	Be	2.0679-06	1.8453-07
LαLβ	**B^+**	33.9557-06	5.0502-07
	Be	7.4798-06	6.6736-06
KβLα	**B^+**	14.9484-06	2.6193-07
	Be ≡		
KαLβ		3.8426-05	3.4291-06
Total	**B^+**	0.6258-04	0.1047-05
	Ref.[10]	0.6253-04	0.1047-05
	Be	0.1537-03	0.4976-04

CONCLUSIONS

For each individual electronic shell the one particle expectation values increase when atom number (Z) increase too. The standard deviation Δr_1 for K- shell is smaller than that found in L-shell since we have Δr_1 determine the diffuse of the one particle radial density distribution $D(r_1)$. The diamagnetic susceptibility for B^+ve for K (^1S) is less than that for L (^1S), KL(^1S), KL(^3S), and total because the diamagnetic susceptibility depends on the radius of 1s and 2s respectively.

REFERENCES

[1] W. Weiss, *Phys. Review*, **1961,** 122, (6).
[2] T. W Valley "Diamagnetic Susceptibilities". San José State University, 15p, **2002**.
[3] E.Z.Liverts, *Computer Physics Communications*, **2010,** 181,206-212.
[4] M.Nasr "Evaluation of X-ray scattering factor for closed shell atoms by using Hartree-Fock and Correlated wave functions" Thesis, **2001**.

[5] E.Hylleraas and S.Skavlem. *Phys. Rev.,* **1950,** 79 (117).
[6] R.Jaber "Study of atomic properties of three electron systems using Hartree-Fock approximation" Thesis, **2012**.
[7] F.K.King, *Phys. Review A*, **1991,** 43(70).
[8] N.M March, "Self-Consistent Fields in Atoms", 1St edition Pergamon Press Ltd, U.K.**1975.**
[9] M. ShGeorge, " Properties of the Radial Wave Function, PhD. Thesis, Baghdad University, Baghdad P.145, **1997**.
[10] F.W.King , Phys. Review A , **1988,** 38(12) .