High Precision Study of K-Shell Some Atomic Systems

لبعض الانظمة الذرية-Kدراسة عالية الدقة للغلاف

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Abstract

The present paper discuss two variational wavefunctions of K-shell atomic systems $Z = 9 - 18$. The first wavefunction deals with the Zeta-Roothaan-Hartree-Fock while the second one considered a simply correlated wavefunction. Several local properties have studied, for instance, radial correlation density function between the two wavefunctions, electron density at the nucleus, diamagnetic susceptibility, and nuclear magnetic shielding constants. We show how the physical properties for K-shell atoms affected by increasing the atomic number Z. All results are obtained via Mathematica program version 10.1.01.

Key words: Nuclear Magnetic Shielding Constant, Diamagnetic Susceptibility, Single-Zeta wavefunction, and Correlated wavefunctions.

الخلاصة

ناقش البحث الحالي دراسة دالتيين موجيتيين للغلاف K للانظمة الذرية Z=9-18. الدالة الاولى تتعامل مع دالة زيتا-روثان-هارتري-فوك المفردة, بينما الثانية توصف كدالة موجية مترابطة. العديد من الخواص قد تم دراستها, على سبيل المثال, الترابط الالكتروني لكثافة جسيم واحد بين الدالتيين الموجيتيين, كثافة الالكترون في النواة, القابلية المغناطيسية, و ثابت الحجب النووي المغناطيسي. لقد تبين أن الخواص الفيزيائية تتغير بزيادة العدد الذري. جميع النتائج قد تم حسابها بأستخدام برنامج Mathematica النسخة 10.1.01.

كلمات مفتاحية: ثابت الحجب النووي المغناطيسي, السماحية المغناطيسية, دالة زيتا-روثان-هارتري-فوك المنفردة الموجية, و دالة موجية مترابطة.

1. Introduction

The two electron system is a subject that has paved the way for extensive studies of a wide range constituted a good test of quantum mechanics topics [**1-8**]. Schrödinger equation for this system is not able to solve it analytically due to the interaction between two electrons. Therefore, an approximation method was obtained to parametrize the wavefunction [**6-9**]. Indeed, several accurate wavefunctions were obtained from variational calculations, where, most of these wavefunctions describe the exact behavior at electron - electron and electron - nucleus coalescence, for instance, by Slater [**10**], Hylleraas [**6,11**], Kinoshita [**1,12-14**], Chandrasekhar [**15,16**], and Hartree-Fock [**17,18**]. Scientific literature had instigated a broad interest in the different wavefunction of the two electrons subject in order to study the physical properties of atoms. Simply correlated wavefunction of many neutral atoms was suggested [**2**]. The highly accurate correlated wavefunction of [**5**] was introduced by angular configuration-interaction method. In addition, the coulomb correlation between two electrons in atoms were discussed [**4,19,20**]. New optimization for Hylleraas wavefunctions technique was obtained [**21**] to study the electron density and electron-pair density. Using modified configuration-interaction and Slater-type wavefunctions the doubly excited intra-shell states was studied in [**22**]. The atomic properties of K-shell atoms using Hartree-Fock wavefunction were studied in [**23-27**]. To this end, most of these studies were focused on the exponential-type orbital due to the high quality of obtaining electronic wavefunction and can be used the linear-combination-of-atomic-orbitals. So the exponential-type orbitals can be represented by linear combinations of reduced Bessel function, so-called β-functions which have simple Fourier transform [**28,29**]. However, This paper addresses the typical issue of physical properties of K-shell neutral atoms Z=9-18, for instance, radial correlation density function, electron density at nucleus, diamagnetic Susceptibility, and nuclear magnetic shielding constant. For this behavior, two different wavefunctions are studied, the Single-Zeta $\mathfrak{B}$-type orbitals wave function (SZ) [**29**] and simple correlated K-shell wavefunctions [**2**]. Our calculations are obtained numerically by using Mathematica package [**30**].

2. Theory and Wavefunctions

The Rayleigh-Ritz variational method is used to obtain the most exact results of eigenvalues and eigenfunctions of the ground state for two electron system. The non-relativistic Hamiltonian Schrödinger equation for the two electron system has a form [**5**]

$$H=-\frac{\nabla_1^2}{2}-\frac{\nabla_2^2}{2}-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}} \qquad \dots\dots(1)$$

Here, $\nabla_{1,2}^2$ is the Kinetic energy of electron with respect to the coordinate of the two electrons. r_1 and r_2 correspond the distance of the electrons to the nucleus as well as r_{12} is the interelectronic separation. $Z/r_{1,2}$ is the potential attraction energy with Z is nuclear charge, and $1/r_{12}$ represents the interelectronic repulsion energy. Therefore, for ground state neutral atoms Z=9-18, We use Zeta $\mathfrak{B}$-type orbitals wavefunction (SZ) [**28,29**] and simply correlated wavefunction of Refs. [**2**], respectively.

A. $\mathfrak{B}$-Type Orbitals Wavefunction

The total wavefunction of the independent practical model is given by Slater determinant [**32**]

$$\Psi_{HF}(x_1,x_2,..x_n)=|\Phi_1(x_1)\Phi_2(x_2)\dots\Phi_N(x_N)\rangle \qquad \dots\dots(2)$$

With the single electron wavefunction $\Phi_i(x_i)$ and x_i denotes spin-orbital components

$$\Phi_i(x_i)=\phi_i(r_i)\alpha(\delta) \qquad \dots\dots(3)$$

r_i denotes the radial and angular co-ordinate, while $\alpha(\delta)$ is the spin wavefunction. The spatial part $\phi_i(r_i)$ can be written as an expansion in some set of analytic basis functions

$$\phi_{nlm}(r,\theta,\varphi)=\sum_{i=1}^{\kappa}C_{nlm}^{i}\chi_{nlm} \qquad \dots\dots(4)$$

where C_{nlm}^{i} is a coefficient taken to minimize the energy, κ refers to the number of states, and χ_{nlm}represent the radial and angular parts, respectively, and can be defined by the $\mathfrak{B}$-type orbitals which has a form as follow

$$\mathfrak{B}_{q,l}^{m}(\alpha;r,\theta,\varphi)=Nr^{l}Y_l^m(\theta,\varphi)\mathcal{R}(r), \qquad \dots\dots(5)$$

The factor N represents the normalization of the radial part

$$N=\frac{2^{l+q}\alpha^{l+1}}{(l+q)!}\sqrt{\frac{\alpha\,\Gamma(2l+2q+2)\,l!\,\Gamma(l+2q)}{\Gamma(2l+4q)\Gamma(2l+1)}}, \qquad \dots\dots(6)$$

while $\Gamma(x)$ is gamma function and $Y_l^m(\theta,\varphi)$ is the complex or real spherical harmonics

$$Y_l^m(\theta,\varphi)=P_{l|m|}\Theta_m(\varphi), \qquad \dots\dots(7)$$

Here $P_{l|m|}$ are normalized associated Legender functions and for complex spherical harmonics [**2**].

$$\Theta_m(\varphi)=\frac{e^{im\varphi}}{\sqrt{2\,\pi}}, \qquad \dots\dots(8)$$

For real harmonics

$$\Theta_m(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos|m|\varphi, & \text{for m } \geq 0 \\ \sin|m|\varphi, & \text{for m } < 0 \end{cases}. \quad \ldots\ldots(9)$$

$\mathcal{R}(r)$ is the reduced Bessel function [**28,29**] with an integer $q \geq 1$

$$\mathcal{R}(r) = e^{-\alpha r} \sum_{i=0}^{q-1} \frac{\Gamma(q+i)(\alpha r)^{q-i-1}}{\Gamma(q-i)\, i!\, 2^i}. \quad \ldots\ldots(10)$$

It is shown that $\mathfrak{B}$-type orbitals has form of linear combination of Slater-type orbitals (STOs) [**28,29**] due to the simplicity of their Fourier transforms which enables to approximate two-center distributions by a sum of one-center distributions placed at the line connecting the original two-centers [**29,33**]. For the $\mathfrak{B}$-type orbitals calculations of ground state neutral atoms Z=9-18, we consider Single-Zeta $\mathfrak{B}$ function basis sets in Ref. **[29]**.

B. Correlated Wavefunction

Our approach the correlated wavefunction is separated into two parts [**34**]

$$\phi_K^{a,b}(r_1, r_2, r_{12}) = \phi(r_1, r_2) \times \phi^{a,b}(r_{12}), \quad \ldots\ldots(11)$$

The second factor corresponds to the correlation function, $\phi^{a,b}(r_{12})$ that it depends only on r_{12}. This approximation was obtained in Ref. [**11**]. The wavefunction of two particles $\phi(r_1, r_2)$ can be written as

$$\phi(r_1, r_2) = \frac{N\, Z^3}{\pi} \left[\mathrm{e}^{-\mathrm{Z}(r_1 + r_2)} \cosh(\alpha\, r_1) \cosh(\alpha\, r_2) \right], \quad \ldots\ldots(12)$$

The factors $\cosh(\alpha\, r_{1,2})$ correspond to the shielding electron 2 (1) on 1 (2) [**2,35**]. Our modulation in this paper is that the function of two-electron contains a product function rather than a sum of one-electron functions. In particular, we address two types of electron-electron correlation functions. The first one is a generalization of Refs. [**34**]

$$\phi^a(r_{12}) = 1 - \frac{e^{-\lambda_a r_{12}}}{1 + 2\lambda_a}. \quad \ldots\ldots(13)$$

The second electron-electron correlation factor is suggested by Ref. [**36**] which build the exponential directly in the wavefunction

$$\phi^b(r_{12}) = e^{-\varepsilon\, r_{12}} - \frac{1+2\varepsilon}{1+2\lambda_a} e^{-\lambda_b r_{12}}. \quad \ldots\ldots(14)$$

The parameters λ_a, λ_b, and ε are variational parameters which obtained from Refs.[**2,34-36**].

3. Theoretical Considerations for Neutral Atoms $Z = 9 - 18$

The electron-pair radial density function $\rho(r_1, r_2)$ refers to the probability density among N electron, one electron is located at a radius r_1 and the second electron at a radius r_2 simultaneously, $\rho(r_1, r_2)$ is defined by [**37**]

$$\rho(r_1, r_2) = \frac{N(N-1)}{2} r_1^2 r_2^2 \int d\tau_1\, d\tau_2 d\Omega_1 d\Omega_2 \ldots d\boldsymbol{x}_N |\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)|^2, \ldots\ldots(15)$$

where $\boldsymbol{x}_i = (\boldsymbol{r}_i, \tau_i)$ represents the combined position-spin coordinate of the electron i, (r_i, Ω_i) with $\Omega_i = (\theta_i, \varphi_i)$ corresponds to the polar coordinate of the position vector $\boldsymbol{r}_i$.

$$d\Omega_i = \int_0^{2\pi} d\varphi_i \int_0^{\pi} d\theta_i \sin\theta_i, \qquad \ldots\ldots(16)$$

while $d\boldsymbol{x}_N$ is obtained via Ref. [**19,38**]. The factor $N(N-1)/2$ represents the electrons pair normalization. The radial density $\rho(r_1)$ is defined

$$\rho(r_1) = \int_0^{\infty} \rho(r_1, r_2) dr_2. \qquad \ldots\ldots(17)$$

We discuss some physical properties which address as follow as

1. Electron density at the nucleus can be written as [**9,36,39**]

$$\rho(0) = \left[\frac{\rho(r_1)}{4\,\pi\, r_1^2}\right]_{r_1 \to 0}. \qquad \ldots\ldots(18)$$

2. Radial electron correlation density is the difference between Zeta-Roothaan-Hartree-Fock (ZRHF) wavefunction Eq. 5 and simply correlated wavefunction Eq. 11 toghther with Eqs. (13) and (14), yielding

$$\Delta\rho(r_1) = \rho(r_1)^a - \rho(r_1)^{ZRHF}, \qquad \ldots\ldots(19)$$
$$\Delta\rho(r_1) = \rho(r_1)^b - \rho(r_1)^{ZRHF}, \qquad \ldots\ldots(20)$$

Where $\rho(r_1)^a$ and $\rho(r_1)^b$ correspond the radial density function for the one-particle of Eq. 11.

3. Diamagnetic Susceptibility is applied to obtain the elastic-scattering cross section of fast electrons from atoms at zero scattering angle, however, diamagnetic susceptibility $\mathcal{D}$ can be written as [**39**]

$$\mathcal{D} = -\frac{\alpha^2}{6}\sum_{i=1}^{2}\int_0^{\infty} \rho(r_1) r_i^2, \qquad \ldots\ldots(21)$$

with the fine structure constant $\alpha = 7.297353 \times 10^{-3}$a. u..

4. Nuclear magnetic shielding constant [**39,40**]

$$\mathcal{NM} = -\frac{\alpha^2}{3}\sum_{i=1}^{2}\int_0^{\infty} \rho(r_1) r_i^{-1}, \qquad \ldots\ldots(22)$$

4. Results and Discussion

We consider Single-Zeta-Beta function basis sets which are obtained by [**29**] for Zeta-Roothaan-Hartree-Fock wavefunction Eq. 5 and we use Ref. [**2**] for simply correlated wavefunction Eqs. 11, 13, and 14.

Figure 1. shows the electron correlation for the radial density which defined in Eqs. 19 and 20, where $\rho(r_1)^{ZRHF}$ corresponds to the radial density of the Zeta-Roothaan-Hartree-Fock wavefunction Eq. 5, while $\rho(r_1)^a$ and $\rho(r_1)^b$ correspond to the radial density of simply correlated wavefunction Eqs. 19 and 20, respectively. We see these function Eqs. 19 and 20 to be positive for small and medium values r_1 and negative for the rest. Due to the correlation leads to increase the probability density of finding the electrons at opposite sides of the nucleus in order to increase the electron-electron distance between them and to eliminate the electrostatic energy among the electrons.

Table 1. discuss the electron density at the nucleus of the K-shell atomic systems $Z = 9 - 18$ for different wavefunctions. According to the coulomb attraction force, we see how $\rho(0)$ in Eq. 18, increase by increasing the atomic number Z. In particular, one could the accuracy of the three wavefunctions densities of table 1 and due to the comparison between these wavefunctions, we can

see that the densities obtained via Eq. 5 are smaller than the values of the other densities at $r_1 \longrightarrow 0$. Indeed, table 1 shows the diamagnetic susceptibility, and nuclear magnetic shielding constants for K-shell atomic systems $Z = 9 - 18$ as well as for different wavefunction. Due to the force between the protons and electrons, we can see that the D in Eq. 21 decreases by increasing the atomic number Z. In particular, the nuclear magnetic shielding constants increase by increasing the atomic number Z.

5. Conclusions

We have studied the local properties for K-shell of some electronic systems. Two different wavefunctions have considered and discussed in detail. Our results indicate how the physical properties behave for K-Shell electronic systems for Zeta-Roothaan-Hartree-Fock and simply correlated wavefunctions, respectively. We have shown that the diamagnetic susceptibility and nuclear magnetic shielding constants decreases (increases) by increasing the atomic number Z.

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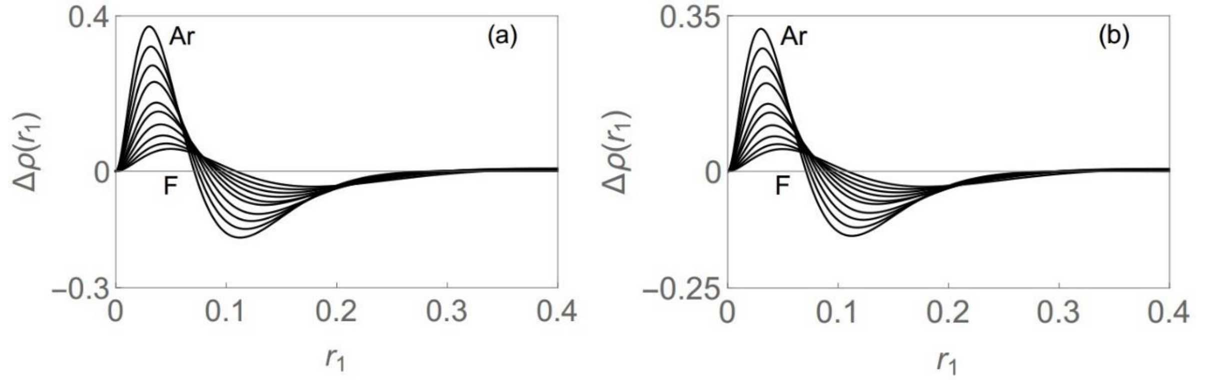

Figure 1. Radial density correlation for K-shell of electronic systems $Z = 9 - 18$. Part (a) describes $\Delta\rho(r_1) = \rho(r_1)^a - \rho(r_1)^{ZRHF}$, while part (b) represents $\Delta\rho(r_1) = \rho(r_1)^b - \rho(r_1)^{ZRHF}$.

Table 1. density at the nucleus $\rho(0)$, Diamagnetic susceptibility, and nuclear magnetic shielding constant for for K-shell of electronic systems $Z = 9 - 18$. which obtained via Single-Zeta-Roothaan-Hartree-Fock Eq. (5) and simply correlated wavefunction Eq. (11) in combining Eqs. (13) and (14), respectively.

Z	$\rho(0)$			$D \times 10^{-7}$ in unit $cm^3\,mol^{-1}$			$\mathcal{NM} \times 10^5$		
	$\mathfrak{B}$TOs	$\phi(r_1,r_2)\phi_K^a$	$\phi(r_1,r_2)\phi_K^b$	$\mathfrak{B}$TOs	$\phi(r_1,r_2)\phi_K^a$	$\phi(r_1,r_2)\phi_K^b$	$\mathfrak{B}$TOs	$\phi(r_1,r_2)\phi_K^a$	$\phi(r_1,r_2)\phi_K^b$
9	32.0104	34.0008	33.9905	7.24719	7.28097	7.27812	30.4713	30.7297	30.7249
10	44.3335	46.903	46.9076	5.83252	5.84966	5.84738	33.9657	34.2544	34.249
11	61.7171	62.81	62.7809	4.80638	4.80901	4.80718	37.4135	37.7613	37.7553
12	80.3563	81.8375	81.8298	4.02995	4.0186	4.01715	40.8535	41.2844	41.2775
13	102.407	104.617	104.517	3.42753	3.40806	3.40679	44.2924	44.8078	44.8006
14	128.225	130.926	131.056	2.9498	2.92579	2.92476	47.7378	48.3368	48.3288
15	158.056	161.806	161.619	2.56529	2.53923	2.53833	51.1835	51.8648	51.8563
16	192.201	196.497	196.492	2.2512	2.2248	2.22374	54.6358	55.3897	55.3837
17	230.957	236.699	235.989	1.99133	1.96462	1.96394	58.0776	58.9231	58.9137
18	274.618	281.93	281.162	1.7739	1.74755	1.74719	61.5263	62.4563	62.4431