

Radial Atomic Properties of Excited States for Beryllium Atom ($1s^2 2s ns$) (1s)

Ruqaya Jabir Hadi¹, Ali Abid Abojassim¹, Laith Najam²

¹Department of Physics, College of Science, Kufa Univ., Kufa, Iraq

²Department of Physics, College of Science, Mosul Univ., Mosul, Iraq

Email address:

ali.ahammedawi@uo.kufa.edu.iq (A. A. Abojassim)

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Abstract: Some radial atomic properties of Be-atom in different excited states ($1s^2 2s 3s$, $1s^2 2s 4s$, $1s^2 2s 5s$) (1s) have been obtained using two electron density function $\Gamma(r_1, r_2)$ in order to solve Hartree-Fock equations using Slater type orbitals using partitioning technique within the individual electronic shells of different configuration of Be-atom in position space. Radial expectations values for one electron $\langle r_1^m \rangle$ and two electrons $\langle r_1^m \cdot r_2^m \rangle$, correlation coefficients τ_r , electron density at the nucleus $\rho(0)$, the nuclear magnetic shielding constant σ_d , and The diamagnetic susceptibility χ_d have been calculated for these states of the same atom.

Keywords: Hartree-Fock-Roothaan Method, Slater Type Orbitals, Two Electron Density Function, Radial Expectation Values, The Nuclear Magnetic Shielding Constant

1. Introduction

The Hartree-Fock-Roothaan (HFR) is one of the approximated methods for solving multi electron systems problem and it is powerful method for studying atomic and molecular systems not only for ground state but also for excited states. In this literature the radial part of one electron basis is expanded in terms of Slater type orbital (STOs) defined by [1]

$$\chi_{nlm_1}(\xi, r) = (2\xi)^{n+\frac{1}{2}} [(2n)!]^{-\frac{1}{2}} r^{n-1} \exp(-\xi r) Y_{lm_1}(\theta, \phi) \quad (1)$$

Here, $\xi_i > 0$ is the orbital exponent. The quantity n occurring in eq. (1) is a positive principal quantum number of (STO). The determination of nonlinear parameters n and ξ is very important for describing the atomic orbitals.

2. Theory

Most of the physically properties of a multi electron system can be calculated from the two-particle reduced density matrix $\Gamma(x_m, x_n)$, without reference to the wavefunction ψ . It contains all the necessary information to compute the energy and many properties of the atoms. It can be gained by integrating the spin and spatial coordinates

of all electrons except two electrons (m, n) from the N -particle density matrix, so the two-electron reduced density matrix $\Gamma(x_1, x_2)$ given by [2, 3].

$$\Gamma(x_1, x_2) = \frac{N(N-1)}{2} \int \dots \int |\psi(x_1, x_2, \dots, x_N)|^2 dx_3 \dots dx_N \quad (2)$$

Where $x_i = (r_i, s_i)$ combined space and spin variable with $s = \alpha$ (spin up) or β (spin down). $\frac{N(N-1)}{2}$ represents the number of electron pairs which can be obtained by integrating the second-order reduced density matrix, so $\Gamma(x_1, x_2)$ is normalized to the number of independent electron pairs within the system as [4,5].

$$\iint \Gamma(x_1, x_2) dx_1 dx_2 = \frac{N(N-1)}{2} \quad (3)$$

The density for the individual electronic shells is obtained by partitioning Γ into its pair-wise components (i, j), where (i, j) labels the occupied normalized spin-orbitals ϕ in the HF description, the two electron density can be written as [6,7].

$$\Gamma_{\text{HF}}(x_1, x_2) = \sum_{i < j=1}^N \Gamma_{ij}(x_1, x_2) \quad (4)$$

$$\Gamma_{ij}(x_1, x_2) = 1/2 \sum_{i < j=1}^N [\phi_i(x_1)\phi_j(x_2) - \phi_j(x_1)\phi_i(x_2)]^2 \quad (5)$$

For Be -atom the number of electron pairs is

$$\frac{N(N-1)}{2} = 6 \tag{6}$$

3. Expectation Values

Expectation value for one-electron $\langle r_1^m \rangle$ is determined by the following expression [8].

$$\langle r_1^m \rangle = \int_0^\infty D(r_1) r_1^m dr_1 \tag{7}$$

Where m integer number ($-2 \leq m \leq 2$). From $\langle r_1^{-2} \rangle$ leads to evaluate the correlation coefficient. The radial expectation value $\langle r_1^{-1} \rangle$ leads to the electron-nuclear potential energy $\langle V_{en} \rangle$ and the nuclear magnetic shielding constant σ_d , from $\langle r_1^2 \rangle$, we determined the atomic diamagnetic susceptibility χ_d , $\langle r_1^1 \rangle$ represented the distance between nucleus and the electron.

$D(r_1)$ is the one-electron radial density function which represents the probability density function to finding an electron at a distance between r_1 and $r_1 + dr_1$ from the coordinate origin (i.e nucleus). The single-electron radial density $D(r_1)$ is obtained from integration over two–electron radial density function $D(r_1, r_2)$ and defined as [9,10],

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \tag{8}$$

Where $D(r_1, r_2)$ is the two-electron radial density function and represents the probability density that one electron is located at a radius r_1 and the other electron at a radius r_2 simultaneously. The two-electron radial density function is given by [11].

$$D(r_1, r_2) = \iint \Gamma(r_1, r_2) r_1^2 r_2^2 ds_1 ds_2 d\Omega_1 d\Omega_2 \tag{9}$$

$$d\Omega_i = \sin \theta_i d\theta_i d\phi_i$$

Where Ω_i is the solid angle.

Two particle expectation value $\langle r_1^m r_2^m \rangle$ is defined as [12].

$$\langle r_1^m r_2^m \rangle = \int_0^\infty \int_0^\infty D(r_1, r_2) r_1^m r_2^m dr_1 dr_2 \tag{10}$$

3.1. Nuclear Magnetic Shielding Constant σ_d

The nuclear magnetic shielding constant is determined from the formula [13].

$$\sigma_d = \frac{1}{3} \alpha^2 \langle \psi | \sum_{i=1}^n (r_i)^{-1} | \psi \rangle \tag{11}$$

Where r_i is the distance from the nucleus to the electron in unit of atomic unit. and (α) fine structure constant $\alpha = \frac{1}{c} \cong \frac{1}{137.036}$ in the atomic units the inner electronic shells shield the external ones thus giving a smaller effective nuclear charge for the outer electrons. the predominant contribution of the S atomic orbitals, and the decreasing relative contribution of the external orbitals as compared to the inner one[14,15].

3.2. The Diamagnetic Susceptibility χ_d

The magnetization M of a substance is proportional to the magnetizing (external) magnetic field B , thus $M = \chi_d B$. The

proportionality factor is the magnetic susceptibility (χ_d). The vast majority of substances have negative magnetic susceptibility (are diamagnetic), or positive, which can be paramagnetic substances [16]. The diamagnetic susceptibility is defined by relation[17]:

$$\chi_d = -\langle r^2 \rangle / (6c^2) \tag{12}$$

3.3. Electron Density at the Nucleus $\rho(o)$

The electron density at the nucleus can be evaluated using the following form [18].

$$\rho(o) = \left[\frac{D_0(r)}{4\pi r^2} \right]_{r \rightarrow 0} \tag{13}$$

3.4. Correlation Coefficients τ_r

The correlation coefficients τ_r are similar to those used in classical statistics. for two electron shell they are defined as [19].

$$\tau_r = \frac{\langle r_1^{-1} r_2^{-1} \rangle - \langle r_1^{-1} \rangle \langle r_2^{-1} \rangle}{\langle r_1^{-2} \rangle - \langle r_1^{-1} \rangle^2} \tag{14}$$

This quantity is restricted by the value $-1 \leq \tau_r \leq +1$, $\tau_r = 1$ ($\tau_r = -1$) means perfect positive (negative) correlation and $\tau_r = 0$ means either non-correlated variables or for independent variables. For the atomic systems non-correlated variables means that the position vectors of any pairs of particles are orthogonal while independent variables means that the diagonal term of the two particle density matrix is the product of the one particle distribution functions[20]. In these systems $\tau_r = 0$ for inner shell ($K\alpha K\beta$)-shell for different excited states.

4. Results and Discussion

Different excited states ($1s^2 2s ns$) ($1s$) of Be-atom where $n=3,4,5$ have been analyzed and some atomic properties have been calculated, the one electron expectation value $\langle r_1^m \rangle$, two electron expectation values $\langle r_1^m r_2^m \rangle$, the nuclear magnetic shielding constant σ_d , the diamagnetic susceptibility χ_d , the electron density at the nucleus $\rho(o)$ and radial correlation coefficient τ_r , it should be mentioned that all numerical calculations have been performed in the Hartree-Fock frame work where in these systems there are six shells, the shells of state $1s^2 2s 3s$ are ($K\alpha K\beta$, $L\alpha M\beta$ $L\alpha M\beta$ $K\alpha L\alpha$, $K\alpha M\beta$, $K\alpha M\beta$, $K\beta M\beta$), the shells of state $1s^2 2s 4s$ are ($K\alpha K\beta$, $L\alpha N\beta$ $K\alpha L\alpha$, $K\beta L\alpha$, $K\alpha N\beta$, $K\beta N\beta$) while the shells of state $1s^2 2s 5s$ are ($K\alpha K\beta$, $L\alpha O\beta$ $K\alpha L\alpha$, $K\beta L\alpha$, $K\alpha O\beta$, $K\beta O\beta$). Table (1) shows the calculated one electron expectation values for studied systems. Table (2) represents expectation values for two electrons, table (3) represents the nuclear magnetic shielding constant σ_d , table (4) shows the diamagnetic susceptibility χ_d , table (5) represents the electron density at the nucleus $\rho(o)$ and table (6) represents the radial correlation coefficient τ_r .

Table 1. One particle expectation value $\langle r_1^m \rangle$ for Be atom in different excited states for each individual electronic shell and for total system.

States	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$
1s ² 2s 3s				
KαKβ	27.75753	3.68200	0.41507	0.23314
LαMβ	0.79178	0.38587	5.05073	37.46877
KαLα ≡ Kβ Lα	14.65327	2.15501	1.32575	3.23864
KαMβ ≡ K β Mβ	13.89552	1.91287	4.14005	34.46340
Total	14.27448	2.3393	2.73290	18.88099
1s ² 2s 5s				
KαKβ	27.76139	3.68232	0.41501	0.23306
LαNβ	0.74257	0.34448	9.37440	155.07254
KαLα ≡ Kβ Lα	14.62012	2.14798	1.35012	3.48410
KαNβ ≡ K β Nβ	13.86866	1.87880	8.43937	151.82462
Total	14.24692	2.01339	4.89473	77.65384
1s ² 2s 5s				
KαKβ	27.76227	3.68239	0.41500	0.23304
LαOβ	0.76027	0.32841	15.16035	442.67004
KαLα ≡ Kβ Lα	14.61441	2.14634	1.35345	3.57375
KαOβ ≡ K β Oβ	13.88518	1.86453	14.22045	439.26630
Total	14.25362	2.00543	7.78719	221.43053

Table 2. Two particles expectation values $\langle r_1^m \cdot r_2^m \rangle$ for Be atom in different excited states for each individual electronic shell and for total system.

States	$\langle r_1^{-2} \cdot r_2^{-2} \rangle$	$\langle r_1^{-1} \cdot r_2^{-1} \rangle$	$\langle r_1^1 \cdot r_2^1 \rangle$	$\langle r_1^2 \cdot r_2^2 \rangle$
1s ² 2s 3s				
KαKβ	770.48071	13.55715	0.17228	0.05436
LαMβ	0.07134	0.09052	17.69746	458.87544
KαLα	10.54599	2.03443	0.91357	1.41625
Kβ Lα	75.43966	2.59015	0.94299	1.49531
KαMβ	0.68175	0.52690	3.26446	16.01543
K β Mβ	1.26023	0.53157	3.26463	16.01557
Total	143.07995	3.22179	4.3759	82.31206
1s ² 2s 4s				
KαKβ	770.69451	13.55949	0.17224	0.05432
LαNβ	0.03176	0.04641	37.93689	2263.04675
KαLα	10.18928	1.99506	0.93435	1.53176
Kβ Lα	71.92765	2.52409	0.96244	1.60763
KαNβ	0.58003	0.27882	6.83274	70.71471
K β Nβ	0.24606	0.27609	6.83263	70.71453
Total	142.27822	3.11333	8.94522	401.27828
1s ² 2s 5s				
KαKβ	770.74392	13.56003	0.17223	0.05431
LαOβ	0.01610	0.02861	64.71947	6825.47135
KαLα	10.10227	1.98542	0.93726	1.57385
Kβ Lα	71.09147	2.50810	0.96503	1.64889
KαOβ	0.29407	0.17178	11.63081	204.68232
K β Oβ	0.11577	0.17031	11.63075	204.68221
Total	142.0606	3.07071	15.00926	1206.35216

Table 3. The Nuclear magnetic Shielding Constant for Be atom in different excited states for each individual electronic shell and for total system.

states	shell	$\sigma_a \cdot 10^{-5}$
1s ² 2s 3s	KαKβ	6.53572
	LαMβ	68.49301
	KαLα ≡ Kβ Lα	3.82524
	KαMβ ≡ K β Mβ	3.39543
	Total	14.91168
1s ² 2s 4s	KαKβ	6.53628
	LαNβ	61.14671
	KαLα ≡ Kβ Lα	3.81276
	KαNβ ≡ K β Nβ	3.33495
	Total	13.66307
1s ² 2s 5s	KαKβ	6.53641
	LαOβ	58.29404
	KαLα ≡ Kβ Lα	3.80984
	KαOβ ≡ K β Oβ	3.30962
	Total	13.17823

Table 4. Diamagnetic Susceptibility for Be atom in different excited states for each individual electronic shell and for total system.

states	shell	$-\chi_d \cdot 10^{-3}$
1s ² 2s 3s	KαKβ	0.00207
	LαMβ	0.33254
	KαLα ≡ Kβ Lα	0.02874
	KαMβ ≡ K β Mβ	0.30587
Total		0.167305
1s ² 2s 4s	KαKβ	0.00207
	LαNβ	1.37630
	KαLα ≡ Kβ Lα	0.03092
	KαNβ ≡ K β Nβ	1.34748
Total		0.68919
1s ² 2s 5s	KαKβ	0.00207
	LαOβ	3.92879
	KαLα ≡ Kβ Lα	0.03172
	KαOβ ≡ K β Oβ	3.89858
Total		1.31548

Table 5. Electron density at the nucleus for Be atom in different excited states for each individual electronic shell and for total system.

states	shell	$\rho(o)$
1s ² 2s 3s	KαKβ	17.12857
	LαMβ	0.43723
	KαLα ≡ Kβ Lα	8.99840
	KαMβ ≡ K β Mβ	8.54727
Total		8.77619
1s ² 2s 4s	KαKβ	17.13132
	LαNβ	0.38521
	KαLα ≡ Kβ Lα	8.97729
	KαNβ ≡ K β Nβ	7.94865
Total		8.56140
1s ² 2s 5s	KαKβ	17.13193
	LαOβ	0.63340
	KαLα ≡ Kβ Lα	8.97901
	KαOβ ≡ K β Oβ	13.25693
Total		10.37287

Table 6. Correlation coefficients for Be atom in different excited states for each individual electronic shell and for total system.

states	shell	$-\tau_r$
1s ² 2s 3s	LαMβ	0.65327
	KαLα	0.56992
	Kβ Lα	0.55006
	KαMβ	0.80097
	K β Mβ	0.80097
Total		0.67504
1s ² 2s 4s	LαNβ	0.74327
	KαLα	0.53481
	Kβ Lα	0.51791
	KαNβ	0.79887
	K β Nβ	0.79887
Total		0.67875
1s ² 2s 5s	LαOβ	0.7758
	KαLα	0.51355
	Kβ Lα	0.49762
	KαOβ	0.80403
Total		0.80403
Total		0.67901

5. Conclusion

This paper shows the effect of radial expectation values $\langle r_1^m \rangle$ of Be-atom in its excited states (1s² 2s ns) where n=3,4,5 to calculate some atomic properties for these systems. When m= -1 this leads to calculate the nuclear

magnetic shielding constant σ_d , when $m = 1$ this means the expectation value for the distance between an electron and the nucleus and also leads to determine the correlation coefficients τ_r and when $m = 2$ this leads to calculate The diamagnetic susceptibility χ_d using Hartree-Fock approximation.

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