Evaluation And Comparison Of The Configuration Potential Energy Calculation For Be-Atom In Position Space

Assist Lecturer Mayada J.AL-Sharaa
Misan University - College of Science

abstract

In the present work studies the theoretically the potential energy expectation value ⟨V⟩ for beryllium atom and like ions for different excited states ($\mathbf{1S^2 2S^1\, nS^1}$) , ($\mathbf{1S^2 2S^1\, nP^1}$) (where Z = 4. 13) and calculate the difference between each state to the same level , was used in this study wave function Hartree – Fook and the results contained in this search match with the published results of Hartree – Fook in 2003 (source 25) . been taking values of (n = 4, 5) to the($\mathbf{1S^2 2S^1\, nS^1}$) state and (n = 2, 3) of the ($\mathbf{1S^2 2S^1\, nP^1}$) state . The computer system Mathcad (Ver 2001i) is used in the present calculations after designing the required program.

تقييم ومقارنة لحساب تكوين الطاقة الكامنة ذرة البريليوم والايونات المشابه لها في الفضاء المكاني

الخلاصة :

البحث الحالي يدرس نظرياً القيمة المتوقعة للطاقة الكامنة ⟨V⟩ لذرة البريليوم والايونات المشابهة لها حيث (Z=4…13) للحالات ($\mathbf{1S^2 2S^1\, nS^1}$)،($\mathbf{1S^2 2S^1\, nP^1}$) وحساب الفرق بين كل حالة لنفس المستوي ، استعملت في هذا الدراسة الدالة الموجية لهارتري –فوك وكانت النتائج المستنتجة في هذا البحث مطابقة مع النتائج المنشورة لدالة هارتري –فوك عام 2004 (مصدر 25).تم اخذ قيم لـ (n=4,5) للحالة ($\mathbf{1S^2 2S^1\, nS^1}$) و (n=2,3) للحالة ($\mathbf{1S^2 2S^1\, nP^1}$) ، تم استعمال نظام حاسوبي ماثكاد Mathcad (Ver 2001i) في حسابات البحث بعد أن تم تصميم البرامج المطلوبة.

Keywords: Energy expectation value, potential energy expectation value, excited states, Hartree- Fock approximation.

1- Introduction

Hartree-Fock theory is essential to much of electronic structure theory. It is the basis of molecular orbital (MO) theory, which hypothesizes that each electron's motion can be described by a single-particle function (orbital) which does not rely evidentially on the simultaneous motions of the other electrons[1]
Hartree -fock atomic wave function is appropriate for many different applications in electronic structure theory . the HF method has taken a central role in studies of atomic and molecular electronic .
Hartree- Fock theory is widely applied for various accounts of the characteristics of multiple electronic systems as well as the calculated excited states are not only ground state. Hartree-Fock theory often supplies a good commencement point for more elaborate theoretical methods which are better approximations to the electronic Schrödinger equation. Hartree-Fock theory was developed to solve the electronic Schrodinger equation that results from the time-independent Schrodinger equation[2]

Theory:

To calculate the potential energy expectation value $\langle V\rangle$ for beryllium atom and like ions for different excited states, which is equal the sum of the energy attraction of electrons with the nucleus and repulsion energy electrons with each other[3] ,which are proportional to the expectation values $\langle r_i^{-1}\rangle$ and $\langle r_{ij}^{-1}\rangle$ respectively. Therefore we may write[4,5,6]

$$\langle V\rangle = -Z\sum_{i}^{N}\langle r_i^{-1}\rangle + \sum_{i<j}^{N}\langle r_{ij}^{-1}\rangle \qquad (1)$$

where Z is the atomic number and energy is in atomic units (a.u.).

The one particle expectation value $\langle r_i^{n}\rangle$ defined as the probability of the electron presence at a certain point for the nucleus.[7,8]
When n = -1 is employed in determination of expectation values of electronic-nuclear attraction potential energy is given in the following equation[9,10,11]

$$\langle r_1^n \rangle = \int_0^\infty D(r_1)\, r_1^n\, dr_1 \qquad (2)$$

Where

$$D(r_1) = \int_0^\infty D(r_1, r_2)\, dr_2 \qquad (3)$$

The one - electron radial density function $D(r_1)$ describes the probability density function of the presence of electrons in their orbits around the nucleus. [12,13]
It can be obtained from the integration of the two-electron radial density function $D(r_1, r_2)$ [14,15,16]

Where

$$D(r_1, r_2) = \int\int \Gamma(r_1, r_2) r_1^2 r_2^2\, d\Omega_1 d\Omega_2 d\sigma_1 d\sigma_2 \qquad (4)$$

$$d\Omega_i = \sin\theta_i\ d\theta_i d\phi_i \qquad (5)$$

WhereΩ_i is the solid angle
The two-electron radial density D(r1,r2) gives the probability density measurement of the presence an electron at a radius r1 and another electron at r2 together at the same time[17,18] . this function is very important in the study of electronic bonding which can tell us about how motion two electron as a result of mutual influence between them [19].

the inter--particle distribution function is the probability distribution of the distance between the electron(1) and electron (2), it is very important in a study for Fermi holes and Cullum, (r12) is the distance between the two electrons, was first presented by Coulson and Nelson for helium atom .The inter-particle distribution function$f(r_{12})$ can be written as follows [20,21,22]:

$$f(r_{12}) = 8\pi^2 r_{12} \begin{bmatrix} \int_0^{r_{12}} r_1 dr_1 \int_{r_1 - r_{12}}^{r_1 + r_{12}} \Gamma(r_1, r_2) r_2 dr_2 + \\ \int_{r_{12}}^{\infty} r_1 dr_1 \int_{r_{12} - r_1}^{r_{12} + r_1} \Gamma(r_1, r_2) r_2 dr_2 \end{bmatrix} (6)$$

Inter - particle expectation value $\langle r_{12}^n \rangle$ is given by the relation [23,24].

$$\left\langle r_{12}^{n}\right\rangle = \int_{0}^{\infty} f(r_{12}) r_{12}^{n} dr_{12} \qquad (7)$$

Where(r_{12}) represents the distance between two-electrons

Results and discussion

The results obtained in the present calculation for the potential energy of ($1S^2 2S^1 nS^1$) state and ($1S^2 2S^1 np^1$) state for Be- like ions up to Z = 13 in excited state are listed in Tables (1 and 2).

The ($1S^2 2S^1 nS^1$) state represented the potential energy for ($n = 4,5$) shell .

Through the results we have obtained and tabulated in Table (1) noted that the potential energy increases by increasing atomic number (Z) in each of The ($1S^2 2S^1 4S^1$) and ($1S^2 2S^1 5S^1$) state .

Table (2) represent the ($1S^2 2S^1 np^1$) state taken ($n = 2,3$) shell . from this table we noted the potential energy increase when the atomic number (Z) increasing for both of ($1S^2 2S^1 2p$) and ($1S^2 2S^1 3p^1$) state.

This result is due to the attraction force of the nucleus to the charge which leads to increase the probability of finding the electron near the nucleus .

we compared our results on the calculation of the potential energy of the ($1S^2 2S^1 4S^1$) ,($1S^2 2S^1 5S^1$), ($1S^2 2S^1 2p^1$) and ($1S^2 2S^1 3p^1$) excited states in Be -like ions (Z - 13) with the other available theoretical results.

The table (3) show the difference between ($1s^2$ $2s^1$ $4s^1$) with ($1s^2$ $2s^1$ $5s^1$) and ($1s^2$ $2s^1$ $2p^1$) with($1s^2$ $2s^1$ $3p^1$) states increases as Z increases.

Table (1): The potential energy expectation values of the excited state in position space for Be - like ions $(1S^2 2S^2\ nS^1)$.

$(1S^2 2S^1\ nS^1)$					
$(1S^2 2S^1\ 4S^1)$			$(1S^2 2S^1\ 5S^1)$		
Atom or ion	Z	$\langle V \rangle$	Atom or ion	Z	$\langle V \rangle$
Be	4	-28.64694536 -28.64724094[25]	Be	4	-28.60881076 -28.60888390[25]
B^{+1}	5	- 47.0728749 -47.07368010[25]	B^{+1}	5	-46.94601018 -46.94639353[25]
C^{+2}	6	-70.12954913 -70.13090362[25]	C^{+2}	6	-69.86774893 -69.86848842[25]
N^{+3}	7	-97.8138131 -97.81584213[25]	N^{+3}	7	-97.37175889 -97.37277056[25]
O^{+4}	8	-130.1247853 -130.12732321[25]	O^{+4}	8	-129.4568222 -129.45826117[25]
F^{+5}	9	-167.0615859 -167.06472044[25]	F^{+5}	9	-166.1227201 -166.12450381[25]
Ne^{+6}	10	-208.62398833 -208.62771715[25]	Ne^{+6}	10	-207.36912214 -207.37124953[25]
Na^{+7}	11	-254.8118160 -254.81614745[25]	Na^{+7}	11	-253.19587801 -253.19835373[25]
Mg^{+8}	12	-305.6249304 -305.62986320[25]	Mg^{+8}	12	-303.60280886 -303.60566334[25]
Al^{+9}	13	-361.0632804 -361.06882084[25]	Al^{+9}	13	-358.59005448 -358.59323102[25]

Table (2): The potential energy expectation values of the excited state in position space for Be - like ions ($\mathbf{1S^2 2S^2\ np^1}$).

$(1S^2 2S^1\ np^1)$					
$(1S^2 2S^1\ 2p^1)$			$(1S^2 2S^1\ 3p^1)$		
Atom or ion	Z	$\langle V \rangle$	Atom or ion	Z	$\langle V \rangle$
Be	4	-28.85517068 -28.83855998[25]	Be	4	-28.67239424 -28.68284709[25]
B^{+1}	5	-48.01944631 -47.97428805[25]	B^{+1}	5	-47.26433909 -47.25832974[25]
C^{+2}	6	-72.18982632 -72.12296073[25]	C^{+2}	6	-70.56930213 -70.56347904[25]
N^{+3}	7	-101.36467641 -101.28204484[25]	N^{+3}	7	-98.60225299 -98.59589122[25]
O^{+4}	8	-135.54497888 -135.44703097[25]	O^{+4}	8	-131.3604006 -131.35317457[25]
F^{+5}	9	-174.72862861 -174.61558038[25]	F^{+5}	9	-168.84255613 -168.83429037[25]
Ne^{+6}	10	-218.91448633 -218.78646069[25]	Ne^{+6}	10	-211.04805982 -211.03865047[25]
Na^{+7}	11	-268.10185055 -267.95892461[25]	Na^{+7}	11	-257.97655666 -257.96594745[25]
Mg^{+8}	12	-322.290302 -322.13252763[25]	Mg^{+8}	12	-309.62785642 -309.61598005[25]
Al^{+9}	13	-381.47956723 -381.30698410[25]	Al^{+9}	13	-366.00174666 -365.98860096[25]

Table(3) : the difference between ($1s^2\ 2s\ 4s$) with (1s 2S 5s) and (1s 2s 2p) with (1s2s3p) state in position space for Be - like ions.

Atom or Ion	Z	□V□□□ (a. u.)	
		$2s^1\ 4s^1)-(1s^2\ 2s^1\ 5s^1)=$	$2s^1\ 2p^1)-(1s^2\ 2s^1\ 3p^1)=$
Be	4	0.038135	0.182776
B^{+1}	5	0.126865	0.755107
C^{+2}	6	0.2618	1.620524
N^{+3}	7	0.442054	2.762423
O^{+4}	8	0.667963	4.184578
F^{+5}	9	0.938866	5.886072
Ne^{+6}	10	1.254866	7.866427
Na^{+7}	11	1.615938	10.12529
Mg^{+8}	12	2.022122	12.66245
Al^{+9}	13	2.473226	15.47782

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