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Research Article

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ABSTRACT

This paper considers correlated form wave function for (C⁺⁴ – Al⁺¹¹) ions. The wavefunction is parametrized by hydrogenic orbital, correlation function, and variationally expansion in r₁, r₂, and r₁₂. To this end, We discuss the radial extracule and intracule densities which are defined the probability of finding the center-of –mass-radius for two electrons and the inter-particle distance, respectively. The moments of the extracule and intracule densities and the radial of two-particle density have studied. we conclude that by increase the atomic number Z, the extracule and intracule densities increase and their position close to the nucleus due to the attraction force between the electron and nucleus. Indeed, the moments increase for the exponent parameter n = –1 with Z increase, while by increasing Z, the moments decrease for n = 1,2.

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INTRODUCTION

The accurate wave function has attracted of many types of research for atomic and molecular physics, for instance, Refs. [1-5]. The variational approach has obtained a good accuracy in the calculation of the two-electronic series [1,6,7] due to the fact that these systems cannot be solved analytically via Schrödinger equation. In particular, the exact atomic Hamiltonian eigenstates of two electronic system has several properties for instance, the moment value of the Hamiltonian has a minimum at the exact wave function, virial theorem, extracule and intracule densities which correspond to the probability density function for a pair of electron having a center of mass vector **R** or relative vector **r**₁₂, respectively [8-11]. Several physical properties were calculated via intracule density, for example, electron correlation problem [1,9,8,12], radial moments and the value of the density at coalescence point that obtained using Hartree-Fock framework [13]. However, this paper we calculate the radial extracule and intracule distribution functions as well as their radial moments for Z=C⁺⁴--Al⁺¹¹ ions. We consider highly compact 4-parameter Hylleraas form for C⁺⁴ – Al⁺¹¹ ions wave function [14,15].

Computational Details

We consider the non-relativistic Hamiltonian Schrödinger equation for the two electrons and an infinitely massive nucleus

of charge Z (in Hartree atomic units, m_e = ħ = e = 4π ε₀ = 1)

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

Here, r₁ and r₂ correspond the distance of the electrons to the nucleus as well as r₁₂ is the interelectronic separation, and ∇_{1,2}² is the Kinetic energy of electron with respect to the coordinate of the two electrons, Z/r_{1,2} is the potential attraction energy with Z is nuclear charge, and 1/r₁₂ represents the interelectronic repulsion energy. We consider a general form for the ground state two-electronic system wave function that having a highly correlated 4-Hylleraas parameters than that defined in Ref. [14,16], yielding

$$\psi(s, t, u) = e^{-\alpha s} \left(1 + \frac{u}{2} e^{-\beta u} \right) Y(s, t, u), \dots \dots (2a)$$

$$Y(s, t, u) = 1 + c_1 s u + c_2 t^2 + c_3 u^2, \dots \dots (2b)$$

where

$$s = r_1 + r_2, \quad t = r_1 - r_2, \quad u = r_{12}, \dots \dots (3)$$

are standard Hylleraas notation. Here α, β, and c₁, c₂, c₃ are obtained variationally by minimizing the energy with respect to them. Furthermore, Eq. (2) satisfies all the cusp conditions, while Eq. (2b) is the correct function of the errors induced by the cusp condition of the term e^{-β u} [17]. For an N-electron system (N ≥ 2), the pair electron motion in atoms is described

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by the radial extracule and intracule densities [2,8,9,12,13,18], yielding

$$D(R) = R^2 \int d\Omega_R \int dr_1 dr_2 \delta \left[R - \frac{r_1 + r_2}{2} \right] \Gamma(r_1, r_2), \quad \dots \dots (4a)$$

$$H(u) = u^2 \int d\Omega_u \int dr_1 dr_2 \delta [u - (r_1 - r_2)] \Gamma(r_1, r_2) \quad \dots \dots (4b)$$

Where $\delta(\mathbf{r})$ is the three-dimensional Dirac delta function, (r, Ω_r) and (u, Ω_u) are the spherical polar coordinates of the vectors \mathbf{u} and \mathbf{R} , respectively, and

$$\Gamma(r_1, r_2) \equiv \binom{N}{2} \int d\sigma_1 d\sigma_2 dx_1 \dots dx_N |\psi(x_1, \dots, x_N)|^2 = \Gamma(s, t, u), \quad \dots \dots (5)$$

is the spin-reduced two-electron density function [18] associated with N -electron wave function $\psi(x_1, \dots, x_N)$ with $x_i \equiv (r_i, \sigma_i)$ is the spin-position coordinates of the electron i . The variable $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ is concerning to the Hylleraas coordinates [19]

$$4R^2 = s^2 + t^2 - u^2 \quad \dots \dots (6)$$

Once the extracule and intracule densities are calculated, the related moments $\langle R^n \rangle$ and $\langle u^n \rangle$ can be written as [2,8,9,12,13,19]

$$\langle R^n \rangle = 4\pi \int_0^\infty dR R^{n+2} D(R), \quad \dots \dots (7a)$$

$$= 4\pi \int_0^\infty du u^{n+2} H(u), \quad \dots \dots (7b)$$

Indeed, the number of pair electrons has form

$$\langle R^0 \rangle = \langle u^0 \rangle = \frac{N(N-1)}{2} \quad \dots \dots (8)$$

Due to the spin-reduced two-electron density function [18], we discuss in detail the two-electron radial density function $D(r_1, r_2)$ which is written as follow as

$$D(r_1, r_2) = r_1^2 r_2^2 \iint d\Omega_1 d\Omega_2 \Gamma(r_1, r_2) \quad \dots \dots (9)$$

RESULTS AND DISCUSSIONS

Our results are obtained via Mathematica Program version 10.1.01. At first, We rewrite Eq. (1) in a form of Hylleraas coordinates. Afterward, We calculate the variational parameters $\alpha, \beta, c_1, c_2, c_3$ in Eq. (2) as shown in table 1, by minimizing the expectation value of the Hamiltonian in term of Hylleraas coordinate with respect to them. The energies E are tabulated in table 1 of the wavefunction Eq. (2) which is in agreement with Ref. [19]. In particular, table 1, mention the influence of the upper shells for the electronic series $C^{+4} - Al^{+11}$ ions.

Table 1 The variational parameter for the electronic series $C^4 - Al^{11}$ ions

Ions	α	β	c_1	c_2	$-c_3$	$-E$ a.u.	$\langle Z u \rangle$	$\langle 1/Z u \rangle$
C^{+4}	5.96481	2.9823	0.352872	0.473621	0.001199	32.321893	2.35187	0.580269
N^{+5}	6.92347	3.4624	0.354839	0.472579	0.001038	44.568127	2.31436	0.590854
O^{+6}	7.87354	3.9438	0.360063	0.466625	0.000918	59.015687	2.28582	0.597928
F^{+7}	8.85427	4.4313	0.377498	0.443947	0.000797	75.235896	2.26745	0.602598
Ne^{+8}	9.96032	4.9811	0.392290	0.425817	0.000702	93.625972	2.25380	0.606119
Na^{+9}	10.7802	5.3921	0.387167	0.43427	0.213027	114.02357	2.21935	0.614433
Mg^{+10}	11.9354	5.9772	0.352464	0.481225	0.198592	136.58932	2.21302	0.616213
Al^{+11}	12.9987	6.5140	0.373865	0.456146	0.202560	160.88725	2.21019	0.617094

Figures 1(a) and 1(b) show the radial extracule and intracule densities Eqs. (4a) and (4b) as a function of the center of mass vector R and the inter-particle distance u for the electronic

series $C^{+4} - Al^{+11}$ ions, respectively. According to the anti-parallel spin component, Fig. 1(a) shows that the probability increases by increasing the distance R and decrease after ($R = 0.164$) for C^{+4} ion and ($R = 0.076$) for Al^{+11} ion, until vanishes. However, the probability to finding the electron occurs at distance ($R = 0.164$) for C^{+4} ion and ($R = 0.076$) for Al^{+11} ion.

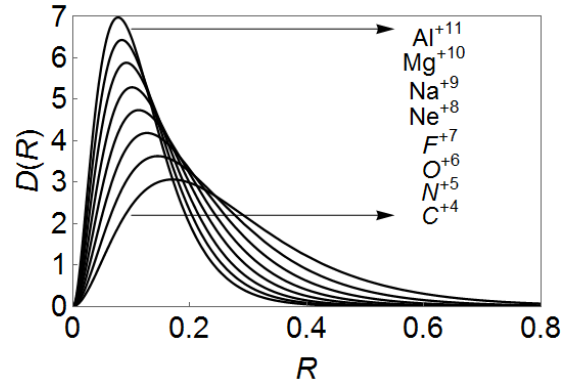


Figure 1(a) The radial extracule density Eq. (4a) versus the center of mass vector R for the electronic series of $C^{+4} - Al^{+11}$ ions.

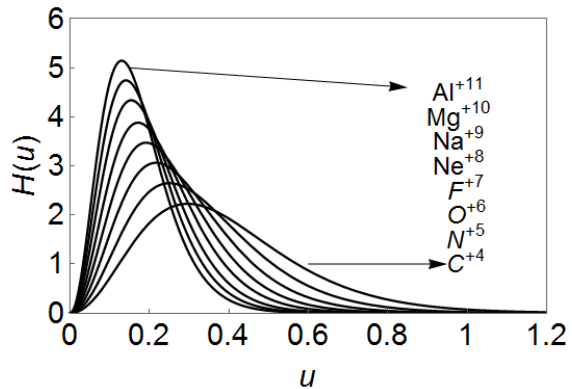


Figure 1(b) The radial intracule density Eq. (4b) versus the inter-particle distance u for the electronic series of $C^{+4} - Al^{+11}$ ions.

Figure 1(b) shows that the probability increases with the increase the inter-particle distance u , then decrease after ($u = 0.302$) for C^{+4} ion and ($R = 0.130$) for Al^{+11} ion. The force between the electron in K-shell and nucleus, both the maximum radial extracule and intracule densities in Figs. 1(a) and 1(b) and their maxima position are close to nucleus by increasing the atomic number Z . Figure 2(a) and 2(b) discuss the moments of extracule and intracule densities $\langle R^n \rangle$ and $\langle u^n \rangle$, respectively, versus to the exponent parameter n which obtain by the correlated wavefunction Eq. (2).

We can see in Fig. 2 that the moments of radial extracule and intracule densities decrease with increase n .

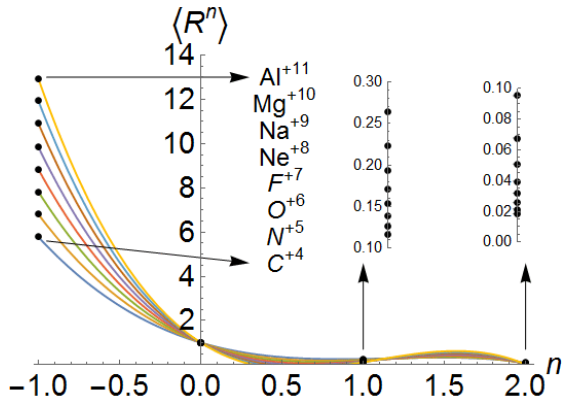


Figure 2(a) The moment values Eq. (7a) for the extracule density as a function of the exponent parameter $n = -1,0,1,2$ for the electronic series of $C^{+4} - Al^{+11}$ ions.

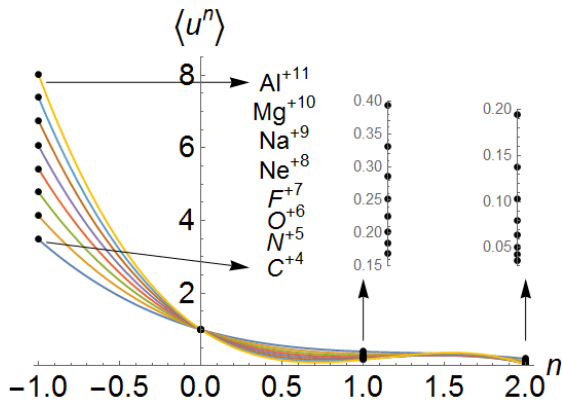


Figure 2(b) The moment values Eq. (7b) for the intracule density as a function of the exponent parameter $n = -1,0,1,2$ for the electronic series of $C^{+4} - Al^{+11}$ ions.

In this paper the exponent parameter n is considered in order to understand the physical properties of $C^{+4} - Al^{+11}$ ions that mentioned in Fig. 2. To this end, Fig. 2(a) $n = -1$ tell us the nuclear magnetic shielding constant. In particular, $n = 0$ refers to the number of pair electrons Eq. (8) and $n = 2$ determine the diamagnetic susceptibility. Indeed, for $n = 1$ to $n = 2$ the moments decrease by increasing Z , this is due to the attraction force of nucleus to the charge which leads to decrease the probability of finding the electron near the nucleus, while for $n = -1$ increases by increasing Z due to strongly attraction force between the nucleus and the electron in the outer shell.

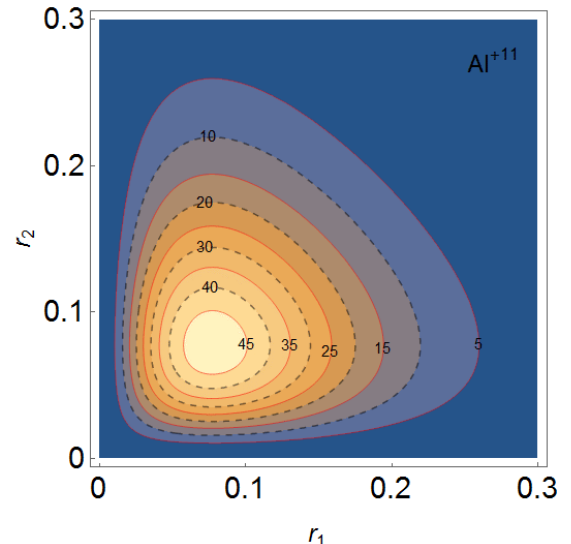
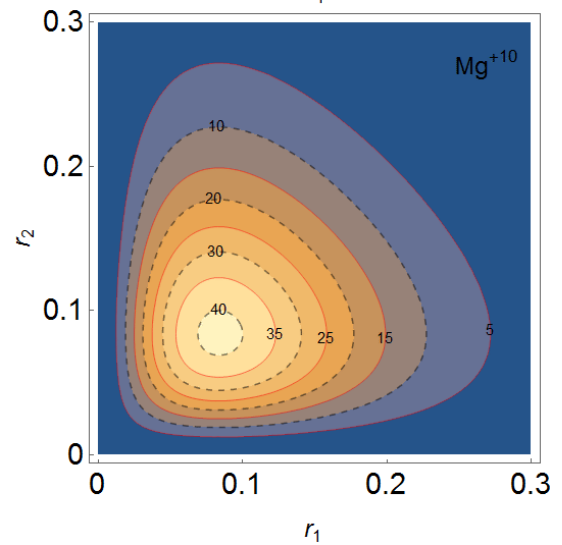
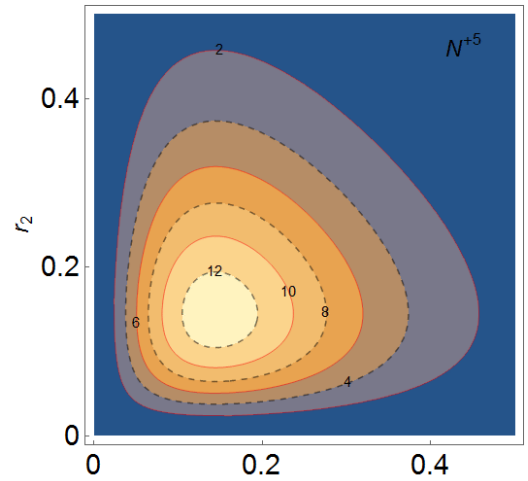
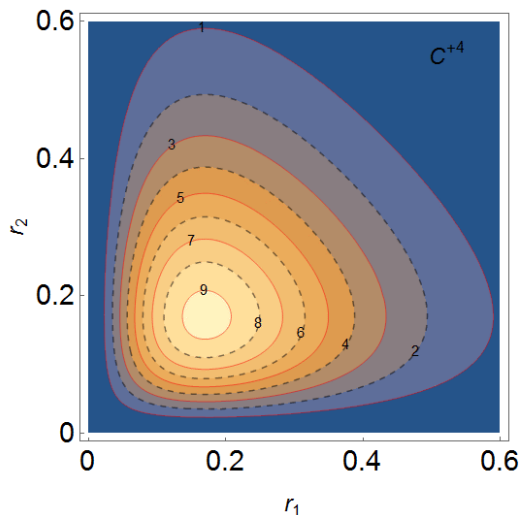


Figure 3 Contours diagram for the radial density function of two electrons Eq. (9) for specific ions C^{+4} , N^{+5} , Mg^{+10} , and Al^{+11} , respectively.

In order to get excellent agreement with Ref. [19], we have to consider more variationally expansion in r_1, r_2 , and r_{12} . Figure 3 read off the radial two electron density $D(r_1, r_2)$ maximum location increase by increasing the Z s shown in contour diagrams and the radial two electron density turn out more diffuses and decreases in magnitude as increases.

CONCLUSIONS

We have studied in detail highly compact 4-parameter correlated wave function. We have discussed the radial extracule and intracule densities for $C^{+4} - Al^{11}$ ions and their moments properties. We showed how the extracule and intracule densities increase by increase the atomic number Z . the radial two electron density turn out more diffuses and decreases in magnitude as increases.

References

1. C. L. Wilson, H. E. Montgomery, Jr., K. D. Sen, D. C. Thompson, 2010, *Electron correlation energy in confined two-electron systems*, Phys. Lett.a, **374**, 4415.
2. T. Koga, 2010, *Electron-pair radial sum and difference moments in atoms*, J. of Mol. Str.: THEOCHEM, **947**, 115.
3. Y. A. Bernard, O. L. Pierre-Franc, and P. M. W. Gill, 2013, *Distribution of $r^{12} \cdot p^{12}$ in quantum systems*, J. Mol. Phys., 111, 2414.
4. P. Koscik and J. K. Saha, 2015, *Ground-State Entanglement Properties of Helium Atom in a Finite Spherical Cavity*, Few-Body Syst., **56**, 645.
5. Rabeet Singh Chauhan and Manoj K. Harbola, 2015, *Highly accurate wave functions for two-electron systems using two parameters*, arXiv: 1506.00912v2.
6. F. E. Harris and V. H. Smith, Jr., 2005, *Highly Compact Wave functions for Two-Electron Systems*, Advances Quantum Chemistry, **48**, 407.
7. U. Kleinekathoefer, S. H. Patil, K. T. Tang, and J. P. Toennies, 1996, *Boundary-condition-determined wave function for the ground state of helium and isoelectronic ions*, Phys. Rev. A, 54, 2840.
8. F. J. Gálvez, E. Buendía, and A. Sarsa, 1999, *Correlated electron extracule densities in position and momentum spaces*, J. Chem. Phys., **111**, 3319.
9. F. J. Gálvez, E. Buendía, and A. Sarsa, 2003, *Electron pair properties for the helium atom from explicitly correlated wave functions*, J. Chem. Phys., **370**, 327.
10. P. M. W. GILL, N. A. BESLEY, and D. P. O'NEILL, 2004, *Wigner Intracule for the Kellner Helium-Like Ions*, Int. J. of Quat. Chem, **100**, 166.
11. J. K. Pearson, P. M.W. Gilla, J. M. Ugaldeb and R. J. Boyd, 2009, *Can correlation bring electrons closer together?*, J. Mol. Phys. 107, 1089.
12. T. Koga, 2007, *Electron–electron radial and angular holes in the Hartree–Fock theory of atoms*, J. Phys. B: At. Mol. Opt. Phys., **40**, 4187.
13. T. Koga; H. Matsuyama, 1997, *Electron - electron coalescence and counterbalance densities of atoms in position and momentum spaces*, Phys. B: At. Mol. Opt. Phys., 30, 5631.
14. C. W. David, 2006, *Compact Singlets S Helium Wave functions (Corrected)*, Chemistry Education Materials.
15. C. Schwartz, 2006, *Experiment and Theory in Computations of the He Atom Ground State*, Int. J. Mod. Phys., **E15**, 877.
16. J. O. Hirschfelder, 1963, *Removal of Electron-Electron Poles from Many Electron Hamiltonians*, J. Chem. Phys. **39**, 3145.
17. R. C. Forrey, 2004, *Compact representation of helium wave functions in perimetric and hyperspherical coordinates*, Phys. Rev. A, **69**, 22504.
18. R. Erdahl and V. H. Smith Jr., *Density Matrices and Density Functionals*, Dordrecht, 1987, pp. 553-581.
19. T. Koga; H. Matsuyama, 1999, *explicitly correlated Extracule densities for two-electron atoms*, Int. J. of Quant. Chem., **74**, 455.

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