Modified Atomic Orbital Calculations of Energy of the \((2s^2 \, ^1S)\) Ground-State, the \((2p^2 \, ^1D)\); \((3d^2 \, ^1G)\) and \((4f^2 \, ^1I)\) Doubly Excited States of Helium Isoelectronic Sequence from \(\text{H}^-\) to \(\text{Ca}^{18+}\)

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Abstract
We report in this paper the ground-state energy \(2s^2 \, ^1S\) and total energies of doubly excited states \(2p^2 \, ^1D\); \(3d^2 \, ^1G\) and \(4f^2 \, ^1I\) of the Helium isoelectronic sequence from \(\text{H}^-\) to \(\text{Ca}^{18+}\). Calculations are performed using the Modified Atomic Orbital Theory (MAOT) in the framework of a variational procedure. The purpose of this study required a mathematical development of the Hamiltonian applied to Slater-type wave function \([1]\) combining with Hylleraas-type wave function \([2]\). The study leads to analytical expressions which are carried out under special MAXIMA computational program. This first proposed MAOT variational procedure, leads to accurate results in good agreement as well as with available other theoretical results than experimental data. In the present work, a new correlated wave function is presented to express analytically the total energies for the \(2s^2 \, ^1S\) ground state and each doubly \(2p^2 \, ^1D\), \(3d^2 \, ^1G\), \(4f^2 \, ^1I\) excited states in the He-like systems. The present accurate data may be a useful guideline for future experimental and theoretical studies in the \((n\ell)\) systems.

Keywords
Modified Atomic Orbital Theory, Variational Calculations, Correlated
Wavefunction, Energies, Ground-State, Doubly Excited States, Helium Isoelectronic Sequence, Atoms and Ions

1. Introduction

The resolution of the Schrödinger equation gives for the ground-state of the Helium atom the value \( E = 108.8 \) eV. The experimental result being equal to \( E_0 = -79.0 \) eV, one conceives that one takes into account the electronic correlation term, overestimating, numerous studies provided evidence of the importance of the electronic correlation in the ground-state and in the doubly excited state of He-like series [3] [4] [5].

For the ground states, energy calculations of Helium isoelectronic sequence are performed by using several correlated wavefunction and an analytical technique calculation. Thus, Moore [6], Radzig and Smirnov [7] and Arnaud [8] measured the ground state energies \( E(1s^2 \, ^1S) \) of two-electron systems with atomic number \( Z (2 \leq Z \leq 10) \). Combining the perturbation theory [9] to the Ritz variational method [10], Sakho et al., [11] set in motion a technic of analytical calculation of the ground state energy \( E(^1S_0) \), the first ionization energy \( J(^1S_0) \) and the radial correlation expectation value \( \langle r_{12}^2 \rangle \) \( ^1S_0 \) for the Helium-like ions from Hydrogen ion \( \text{H}^- \) \( (Z = 1) \) to silicon \( \text{Si}^{12+} \) \( (Z = 14) \). Utpal and Talukdar [12] used an analytical approach to also calculate the ground-state energies of helium isoelectronic sequence from Hydrogen ion \( \text{H}^- \) \( (Z = 1) \) up to the silicon ion \( \text{Si}^{12+} \) \( (Z = 14) \). For some methods using variational wavefunction like Hylleraas’s one, a good approximation of the eigenvalues is obtained when the minima of the function \( \frac{dE}{d\alpha} \), with \( \alpha \) a variational parameter, \( E \) is the energy converges with the increasing values of the dimension \( D \) and when the function \( E = f(\alpha, D) \) exhibits a plateau [2]. For other methods using a non variational wavefunction [13], the ground-state energy of He-like ions is determined by the use of proper core boundary conditions correct behavior for \( r_{12} \rightarrow 0 \) and \( r_{12} \rightarrow \infty \) and by taking recourse to a perturbative method. For some methods using an analytical technique calculation, some authors were interested in the setting in work of calculation techniques permitting one to succeed to an analytical expression of the ground-state energy of the He-like ions. Thus, an analytical calculation for the ground-state energy and radial expectation values of Helium isoelectronic sequence is managed by using a wavefunction of the type of Bhattacharyya [12] [14]. Besides, developing the orbital atomic theory, Slater in [15] introduced the notions of screen constant \( \sigma \) and effective quantum number \( n^* \) for the calculation of the energy of an electronic configuration given containing \( N \) electrons.

On the basis of his theory, Slater expresses analytically the total energy of an atomic system of \( N \) electrons according to \( \sigma \) and \( n^* \) determined from rules that he established. The analytical formula of Slater permits the simple calculation of the ground-state energy of He-like ions for which \( N = 2, \sigma = 0.30 \) and \( n^* = 1 \).
For the doubly excited states in He-like ions, since the early experiment [16] and theoretical explanation [17], Doubly Excited States (DES) of Helium isoelectronic sequence have been the target of a number of theoretical approaches. Greatest attention have been concentrated on studying symmetric DES (nl^2) with excited electrons having equal values of principal quantum number n (intrashell states) where the electronic correlation effect may be predominant [18]. The investigations of the intrashell states of two-electrons systems are advanced and due to the group theoretical method [19] which allowed intrashell states to be approximatively classified and some of these properties studied [20]. Theoretical investigations of (nl^2) doubly excited states are performed by using various method. The projection operator method and group theoretical methods [20] have been used for energies calculations of the 2s^2, 2p^2 states in Helium-like ions. Time independent variational perturbation [21] was applied for total energies calculations of the 2s^2, 2p^2 and 3d^2 states in He, Li^+, Be^{2+} and B^{3+}. The correlation part of the energies for the 2s^2, 2p^2, 3s^2, 3p^2, 3d^2 states in He isoelectronic series have been investigated by using perturbation theory [4]. The Screening Constant by Unit Nuclear charge (SCUNC) method [22] used a semi-empirical procedure to calculate (ns^2) 1S, (np^2) 1D^0 and (Nsnp) 1P^0 excited state of He-like ions. Recently the Modified Atomic Orbital Theory (MAOT) has been applied successfully in the studies of high lying 1^3P^0 of He-like ions [1]. In this paper, we apply the first MAOT variational procedure, to calculate the ground-state energy 2s^2 1S and the total energies of the singlet DES 2p^2 1D, 3d^2 1G and 4f^2 1I of He isoelectronic sequence from H^- to Ca^{18+}. In addition, for the first time in our knowledge, we have also calculated theoretical the screening constant $\sigma_{tho}$ which is compared with experimental Slater screening constant ($\sigma_{exp}$) determined from his rule. Our present procedure leads to analytical expression which are carried out under MAXIMA computational program. Our energies positions are compared to other available theoretical and experimental data.

2. Theory

2.1. Brief Description of the MAOT Formalism

In the framework of Modified Atomic Orbital Theory (MAOT), total energy of (νℓ)-given orbital is expressed in the form [1] [23]:

$$E(\nu\ell) = \frac{1}{\nu^2} \left[ Z - \sigma(\ell) \right]^2$$  \hspace{1cm} (1)

For an atomic system of several electrons $M$, the total energy is given by (in Rydberg):

$$E = \sum_{i=1}^{M} \frac{1}{\nu_i^2} \left[ Z - \sigma_i(\ell) \right]^2$$

With respect to the usual spectroscopic notation \((N\ell, N'\ell') 2S+1L^\pi\), this equation becomes
In the photoionization study, energy resonances are generally measured relatively to the $E_\infty$ converging limit of a given $(2S+1LJ)nl$-Rydberg series. For these states, the general expression of the energy resonances is given by the formula [24] presented previously (in Rydberg units):

$$E_n = E_\infty - \frac{1}{n} \left\{ Z - \sigma_1 \left( 2S+1LJ \right) - \sigma_2 \left( 2S+1LJ \right) \times \frac{1}{n} \right. $$

$$- \left. \sigma_3 \left( 2S+1LJ \right) \times (n-m) \times (n-q) \sum_k f_k(n,m,q,s) \right\}^2 $$

(3)

In this equation $m$ and $q$ ($m < q$) denote the principal quantum numbers of the $(2S+1LJ)nl$-Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_j(2S+1LJ)$-screening constants, $s$ represents the spin of the $nl$-electron ($s = 1/2$), $E_n$ is the energy value of the series limit generally determined from the NIST atomic database, $E_\infty$ denotes the corresponding energy resonance, and $Z$ represents the nuclear charge of the considered element. The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k f_k(n,m,q,s)$ term. The correct expression of this term is determined iteratively by imposing general Equation (3) to give accurate data with a constant quantum defect values along all the considered series. The value of $\alpha$ in the $\sigma_3$ of the last term is fixed to 1 and 2 during the iteration. The quantum defect $\delta$ is calculated from the standard formula

$$E_n = E_\infty - \frac{RZ_{\text{core}}^2}{(n-\delta)^2} \Rightarrow \delta = n - Z_{\text{core}} \sqrt{\frac{R}{(E_\infty - E_n)}} $$

(3 bis)

In this Equation (3 bis), $R$ is the Rydberg constant, $Z_{\text{core}}$ represents the electric charge of the core ion. $Z_{\text{core}}$ is directly obtained by the photoionization process from an atomic $X$ system $X + h\nu \rightarrow X^{p+} + pe^-$

$$f_k = f_k^{(2S+1LJ,n,s,m,q)}$$

are screening constants to be evaluated empirically with $k$ taking the values from 1 to $q$.

$LJ$ denote the considered quantum state ($S, P, D, F, ...$).

2.2. Variational Procedure of Calculations

For the $2s^1S$ ground state and each doubly excited states $2p^1D$, $3d^1G$, $4f^1I$, we constructed the basis wave functions below by combining Slater-type wave function [1] and Hylleraas-type wave functions [2]:

$$\phi_{\text{Slater}}(r_1, r_2) = (r_2)^{\left(\nu - \frac{1}{2}\right)} \times \exp \left( -\frac{Z - \sigma}{\nu \times a_0} \right) \left( r_1 + r_2 \right)^{\nu} \left( r_1 - r_2 \right)^{\nu} \left| r_1 - r_2 \right|^m $$

(4)

We considered parameter
\[ \xi = \frac{Z - \sigma}{\upsilon \times a_0} \]  

(5)

and \( Z, \sigma, \upsilon \) and \( a_0 \) are respectively the nucleus charge number, the screening constant, the principal quantum number and Bohr’s radius

\[ \phi_{\text{kmn}}(r_1, r_2) = (r_1 r_2)^{(\upsilon - 1)} \times \exp\left(-\xi (r_1 + r_2)\right) \left(r_1 - r_2\right)^{\kappa} \left|r_1 - r_2\right|^{\mu} \]  

(6)

With \( \left|r_1 - r_2\right| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}} \)

where \( r_1 \) and \( r_2 \) denote the positions of the two electrons;

\( r_1 \) and \( r_2 \) are respectively used for \( |r_1| \) and \( |r_2| \), \( J, K, M \) are Hylleraas parameters with \( (J, K, M \geq 0) \).

\( J \) takes into account the distance of the two electrons from the nucleus.

\( K \) takes into account the approximation of the two electrons from the nucleus.

\( M \) takes into account the distance between the two electrons.

From Equation (5) the screening constant can be expressed

\[ \sigma = Z - a_0 \upsilon \xi \]  

(7)

The final form of the wave function of the singlet doubly excited state can be written as follow:

\[ \Psi_s(r_1, r_2) = \sum_{jkm} \beta_{jkm} \phi_{jkmn}(r_1, r_2) \]  

(8)

where the coefficients \( \beta_{jkm} \) are determined by solving the Schrödinger equation:

\[ H \Psi_s(r_1, r_2) = E \Psi_s(r_1, r_2) \]  

(9)

where the Hamiltonian operator \( H \) has the form:

\[ H = T + C + W \]  

(10)

\[ T = \frac{-\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) ; \quad C = -\left( \frac{Ze_1}{r_1} + \frac{Ze_2}{r_2} \right) ; \quad W = \frac{e^2}{|r_1 - r_2|} \]  

(11)

where \( T \) is the kinetic energy, \( C \) is the Coulomb potential between the atomic nucleus and the two electrons, \( W \) is the Coulomb interaction between electrons.

In this Equation (11), \( Z \) is the nuclear charge \( \nabla_1 \) is the Laplacian with reference to the coordinates of the vector radius \( r_1 \) which detect the position of the electron 1. \( \nabla_2 \) Laplacian defines the coordinates of the vector radius \( r_2 \) which detect the position of the electron 2 and \( |r_1 - r_2| \) inter-electronic distance.

The representation of the Schrödinger equation on the non-orthogonal basis leads to the general eigenvalue equation [25];

\[ \sum_{jkm} \left( H_{\text{JKMol}} - E N_{\text{JKMol}} \right) = 0 \]  

(12)

With \( J = j + j' \); \( K = k + k' \); \( M = m + m' \)

\[ N_{\text{JKMol}} = \left( \phi_{jkm} \right) \left( \phi_{jkm}^* \right) \]: is the normalization factor  

(13)
\[ H_{\text{JKM}nl} = \langle \phi_{jkmn} | H | \phi_{j'k'm'n'} \rangle \]: is the matrix elements of Hamilton operator (14)

\( E \) is the eigenvalue of the energy

\[ H_{\text{JKM}nl} = T_{jkm, j'k'm'n'} + C_{\text{JKM}nl} + W_{\text{JKM}nl} \] (15)

\( T_{jkm, j'k'm'n'} \): is the matrix elements of the kinetic Energy operator of the two electrons

\( C_{\text{JKM}nl} \): is the matrix elements of the Coulombian interaction Energy operator between the nucleus and the two electrons

\( W_{\text{JKM}nl} \): is the matrix elements of the Coulombian interaction Energy operator between the two electrons

Thus following the form of the basis wave function above (4), we have constructed for each state a special wave function and then calculated the matrix elements \( N_{\text{JKM}nl} \), \( C_{\text{JKM}nl} \), \( W_{\text{JKM}nl} \), \( T_{jkm, j'k'm'n'} \)

**For example on \( 2p^2 \) states:** \( n = \nu = 2; l = 1 \)

The wave function is written as follow:

\[ \phi_{jkmn}(r_1, r_2) = (r_1 r_2) \times \exp(-\xi (r_1 + r_2))(r_1 + r_2) \psi (r_1 - r_2)^\mu | r_1 - r_2 |^\mu \] (16)

The matrix elements of the normalization factor is written as follow:

\[ N_{\text{JKM}21} = \langle \phi_{jkmn} | \phi_{j'k'm'n'} \rangle \] (17)

\[ N_{\text{JKM}21} = \int d^3 r_1 d^3 r_2 \phi_{jkmn}(r_1, r_2) \times \phi_{j'k'm'n'} (r_1, r_2) \] (18)

\[ N_{\text{JKM}21} = \int d^3 r_1 d^3 r_2 (r_1 + r_2)^2 (r_1 + r_2)^\psi (r_1 - r_2)^\mu \times \exp(-2\xi (r_1 + r_2)) \] (19)

With \( \int d^3 r_1 = \int r_1^2 d\theta_1 \sin \theta_1 d\theta_2 \int d\phi_1 = 4\pi \int r_1^2 dr_1 \) \( (i = 1, 2) \) (20)

The matrix elements of the Coulombian interaction Energy operator between the nucleus and the two electrons is written as follow:

\[ C_{\text{JKM}nl} = \langle \phi_{jkmn}(r_1, r_2) | C | \phi_{j'k'm'n'}(r_1, r_2) \rangle \] (21)

\[ C_{\text{JKM}21} = \langle \phi_{jkmn}(r_1, r_2) | -Ze^2 \left( \frac{1}{r_1} + \frac{1}{r_2} \right) | \phi_{j'k'm'n'}(r_1, r_2) \rangle \] (22)

\[ C_{\text{JKM}21} = -Ze^2 \int d^3 r_1 d^3 r_2 \phi_{jkmn}(r_1, r_2) \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \phi_{j'k'm'n'}(r_1, r_2) \] (23)

The matrix elements of the Coulombian interaction Energy operator between the two electrons is expressed as follow:

\[ W_{\text{JKM}nl} = \langle \phi_{jkmn}(r_1, r_2) \left( \frac{1}{r_1 - r_2} \right) | \phi_{j'k'm'n'}(r_1, r_2) \rangle \] (24)

\[ W_{\text{JKM}21} = \int d^3 r_1 d^3 r_2 \phi_{jkmn}(r_1, r_2) \left( \frac{1}{r_1 - r_2} \right) \phi_{j'k'm'n'}(r_1, r_2) \] (25)

The matrix elements of the kinetic Energy operator of the two electrons is ex-
pressed as follow:

\[
T_{jkm, J'K'M'} = \left\langle \phi_{jkm} (r_1, r_2) \left| -\frac{\hbar^2}{2m} \left( \nabla_1 + \nabla_2 \right) \right| \phi_{J'K'M'} (r_1, r_2) \right\rangle \tag{26}
\]

Calculations for the other matrix elements of other states were obtained in the same procedure.

The mathematical development of the Hamiltonian applied to each wave function of each states leads to simplified analytical expressions which are carried out under MAXIMA computational program.

Concerning the screening constant \( \sigma \) and the variational parameter \( \xi \), the procedure is as follow:

From the Slater condition \( 0.3 \leq \sigma \leq 1 \), and taken into account Equation (5), the parameter \( \xi \) can be expressed as follow:

\[
Z - \frac{1}{n} \leq \xi \leq \frac{Z}{n} \tag{27}
\]

In order to obtain the theoretical screening constant \( \sigma_{theo} \), the exponential parameter \( \xi \) and the minimum eigenvalue in which we are interested, the analytical expressions of each matrix elements of each state are carried out by our self MAXIMA computational program.

MAXIMA is a computer algebra system for the manipulation of symbolic and numerical expressions, including differentiation, integration, ordinary differential equations, and matrix elements. MAXIMA yields high precision numeric results by using exact fractions, arbitrary precision integers, and variable precision floating point numbers. Our MAXIMA source code is compiled on windows systems.

At the beginning, the variational parameter \( \xi \) is determined as shown (27). For each value of \( Z \) and \( n \), we know a limited area of the variational parameter \( \xi \). Thus for each value of \( Z \), \( n \) and \( \xi \), the program calculated directly the screening constant \( \sigma \) as shown the Equation (7) and then the eigenvalue \( E \). To obtain the minimum eigenvalue and the theoretical screening constant in which we are interested and quoted in tables 1 - 4, the variational parameter \( \xi \) and the Hylleraas parameters \( (J, K, M) \) are slightly varied that exhibit a plateau for the energy.

### 3. Results and Discussions

The main results of our calculations for the theoretical screening constant, the variational parameter \( \xi \) and energies concerning the \( 1s^2 \, ^1S \) ground-state and the Doubly Excited State for \( 2p^2 \, ^1D, \, 3d^2 \, ^1G \) and \( 4f^2 \, ^1I \) of helium isoelectronic sequence are quoted respectively in Tables 1-4. Our present results are compared with other theoretical calculations and experimental data. Then our results are converted into Rydberg for direct comparison by using the infinite Rydberg 1Ry \( = 0.5 \) a.u \( = 13.605698 \) eV. Table 1 shows a comparison of the present calculation for the \( 1s^2 \, ^1S \) ground-state energy with the experimental data [6] [7] [8], and the theoretical results [9] [10] [11] [12] [15]. In addition the theoretical screening
Table 1. Variational parameter \( \xi \) and ground energies for \( 1s^2 \) \( 1S \) states of Helium isoelectronic sequence. The values are reported in Rydberg (Ry). 1Ry = 13.605698 eV. The screening constant \( \sigma_{\text{theo}} = 0.3101 \).

| \( \text{Theory} \) | \( \xi \) | \( -E^{\text{MAOT}} \) | \( -E^{\text{Sakho}} \) | \( -E^\text{a,b} \) | \( -E^\text{B} \) | \( -E^\text{Slater} \) | \( -E^\text{exp} \) |
|----------------|------|----------------|----------------|----------------|----------------|----------------|----------------|
| \( H^- \) | 0.6899 | 1.0098 | 1.1406 | 1.0164 | 0.9745 |
| He | 1.6899 | 5.7951 | 5.8872 | 5.8071 | 5.8078 | 5.7784 | 5.7799 | 5.7233 | 5.8063 | 5.8071 |
| Li\(^+\) | 2.6899 | 14.5063 | 14.6401 | 14.5593 | 14.5615 | 14.5321 | 14.6049 | 14.4726 | 14.4645 | 14.5593 |
| Be\(^{2+}\) | 3.6899 | 27.2554 | 27.3907 | 27.3113 | 27.3150 | 27.2844 | 27.4260 | 27.2224 | 27.2238 | 27.3120 |
| B\(^{3+}\) | 4.6899 | 43.9813 | 44.1403 | 44.0616 | 44.0690 | 44.0352 | 44.2542 | 43.9720 | 43.9815 | 44.0683 |
| C\(^{4+}\) | 5.6899 | 64.7582 | 64.8904 | 64.8125 | 64.8228 | 64.7860 | 65.0896 | 64.7221 | 64.7449 | 64.8294 |
| N\(^{5+}\) | 6.6899 | 89.5054 | 89.6403 | 89.5624 | 89.5779 | 89.5367 | 89.9314 | 89.4720 | 89.5999 |
| O\(^{6+}\) | 7.6899 | 118.3513 | 118.3908 | 118.2886 | 118.3342 | 118.2872 | 118.7803 | 118.2952 | 118.3834 |
| F\(^{7+}\) | 8.6899 | 151.0853 | 151.1403 | 151.0631 | 151.0903 | 151.0374 | 151.6357 | 150.9721 | 151.2366 |
| Ne\(^{8+}\) | 9.6899 | 187.9563 | 187.8903 | 187.8840 | 187.8477 | 187.8784 | 188.4974 | 187.7221 | 188.0050 |
| Na\(^{9+}\) | 10.6899 | 228.6006 | 228.6395 | 228.6056 | 228.6537 | 228.9797 | 228.4719 |
| Mg\(^{10+}\) | 11.6899 | 273.4513 | 273.3906 | 273.3648 | 273.2877 | 273.7801 | 273.2222 |
| Al\(^{11+}\) | 12.6899 | 322.0992 | 322.1407 | 322.1245 | 322.0378 | 322.5802 | 321.9724 |
| Si\(^{12+}\) | 13.6899 | 374.9353 | 374.8907 | 374.8855 | 374.8855 | 374.8855 | 374.8855 | 374.8855 | 374.8855 |
| P\(^{13+}\) | 14.6899 | 431.4453 |
| S\(^{14+}\) | 15.6899 | 492.1952 |
| Cl\(^{15+}\) | 16.6899 | 556.9453 |
| Ar\(^{16+}\) | 17.6899 | 625.6953 |
| K\(^{17+}\) | 18.6899 | 698.4452 |
| Ca\(^{18+}\) | 19.6899 | 775.1954 |

\( E^{\text{MAOT}} \): Energy \( E \) of the Modified Atomic Orbital Theory (MAOT), present work. \( E^{\text{Sakho}} \) (Sakho, 2006) [11]; \( E^\text{a,b} \) (Pekeris, 1962); \( E^\text{B} \) (Drake, 1988) [9]; \( E^{\text{Slater}} \) (Minkine, 1982) [15]; \( E^\text{exp} \) Experimental data (Radzig, 1985 [7]; Arnaud, 1993) [8]; \( E^\text{f} \) (Moore, 1971) [6]; \( E^\text{f} \) (Utpal and Talukdar, 1999) [12]; \( E^\text{f} \) (Roothaan et al., 1960) [10].

Constant \( \sigma_{\text{theo}} = 0.3101 \) is also presented and agree very good with the experimental screening constant of Slater \( \sigma_{\text{Slater}} = 0.30 \) determined from his rule (\( \sigma_{\text{Slater}} = 0.30 \) for \( 1s^2 \) state, \( n = 1 \)). For \( H^- \) \( (Z = 1) \), our results at \(-1.0098 \) Ry are compared with those of [10] [11] [12], respectively at \(-1.14069 \) Ry; \(-1.01648 \) Ry and \(-0.97459 \) Ry and it can see the good agreement. Comparison indicates that MAOT results agree well with each other up to \( Z = 10 \). For \( 10 < Z \leq 14 \), our results are compared with those of [10] [11] [15]. Comparison indicates that for \( Z = 14 \), our total energy at \(-374.9353 \) Ry agree with [11] at \(-374.89072 \) Ry, with [9] at \(-374.88558 \) Ry, with [15] at \(-375.38022 \) Ry and with [10] at \(-374.72241 \) Ry. Generally, this good agreement enables to expect our results with MAOT calculation for ground-state energy up to \( Z = 20 \) to be accurate.

In Table 2, we presented the theoretical screening constant \( \sigma_{\text{theo}} = 0.3512 \) and reported the value of the variational parameter \( \xi \) and total energies for \( 2p^2 \) \( 1D \)
Table 2. Parameter $\xi$ and total energies $E$ for doubly excited $2p^1 D$ states. The values are reported in Rydberg (Ry). $1 \text{Ry} = 13.605698 \text{ eV}$. The screening constant $\sigma_{\text{theo}} = 0.3512$.

| Element | $\xi_{\text{MAOT}}$ | $E_{\text{SCUNC}}$ | $E_{\text{MAOT}}$ | $E_{\text{Biaye et al.}}$ | $E_{\text{Ray et al.}}$ | $E_{\text{Roy et al.}}$ | $E_{\text{Ho and Bhatia}}$ | $E_{\text{Ivanov and Safronova}}$ | $E_{\text{Hicks and Comer}}$ | $E_{\text{Diehl et al.}}$ |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| H$^{-}$ | 0.3244          | 0.2335          |                 |                 |                 |                 |                 |                 |                 |                 |
| He      | 0.8244          | 1.3481          | 1.4052          | 1.4097          | 1.4266          | 1.4052$^a$      | 1.3728          |                 |                 |                 |
| Li$^+$  | 1.3244          | 3.5398          | 3.5418          | 3.5565          | 3.5110          | 3.5411          | 3.5565          | 3.5396$^f$      | 3.3906          |
| Be$^{1+}$ | 1.8244        | 6.6838          | 6.6788          | 6.6993          | 6.6545          | 6.6751          | 6.6861          | 6.5097          |                 |                 |
| B$^{2+}$ | 2.3244          | 10.8132         | 10.8153         | 10.8403         | 10.7976         | 10.8072         | 10.8160         | 10.6266         |                 |                 |
| C$^{3+}$ | 2.8244          | 15.9892         | 15.9514         | 15.9793         | 15.9455         |                 |                 |                 |                 |                 |
| N$^{4+}$ | 3.3244          | 22.0819         | 22.0885         | 22.1186         | 22.0753         |                 |                 |                 |                 |                 |
| O$^{5+}$ | 3.8244          | 29.1999         | 29.2252         | 29.2568         | 29.2046         |                 |                 |                 |                 |                 |
| F$^{7+}$ | 4.3244          | 37.3396         | 37.3615         | 37.3946         | 37.3350         |                 |                 |                 |                 |                 |
| Ne$^{8+}$ | 4.8244         | 46.5156         | 46.4981         | 46.5327         | 46.4643         |                 |                 |                 |                 |                 |
| Na$^{9+}$ | 5.3244         | 56.6290         |                 |                 |                 |                 |                 |                 |                 |                 |
| Mg$^{10+}$ | 5.8244        | 67.7463         |                 |                 |                 |                 |                 |                 |                 |                 |
| Al$^{11+}$ | 6.3244        | 79.9033         |                 |                 |                 |                 |                 |                 |                 |                 |
| Si$^{12+}$ | 6.8244        | 93.0931         |                 |                 |                 |                 |                 |                 |                 |                 |
| P$^{13+}$ | 7.3244         | 107.2076        |                 |                 |                 |                 |                 |                 |                 |                 |
| S$^{14+}$ | 7.8244         | 122.3587        |                 |                 |                 |                 |                 |                 |                 |                 |
| Cl$^{15+}$ | 8.3244        | 138.4988        |                 |                 |                 |                 |                 |                 |                 |                 |
| Ar$^{16+}$ | 8.8244         | 155.6603        |                 |                 |                 |                 |                 |                 |                 |                 |
| Kr$^{17+}$ | 9.3244         | 173.8364        |                 |                 |                 |                 |                 |                 |                 |                 |
| Ca$^{18+}$ | 9.8244         | 193.0401        |                 |                 |                 |                 |                 |                 |                 |                 |

$E_{\text{MAOT}}$: Energy $E$ of the Modified Atomic Orbital Theory (MAOT), present work. SCUNC (Sahko, 2008) [22]; $E_{\text{Biaye et al.}}$ (Biaye et al., 2005) [2]; $E_{\text{Ray et al.}}$ Experimental data (Ray et al., 1991) [21]; $E_{\text{Roy et al.}}$ (Roy et al., 1997) [26]; $E_{\text{Ho and Bhatia}}$ (Ho and Bhatia, 1991) [27]; $E_{\text{Ivanov and Safronova}}$ Experimental data (Ivanov and Safronova, 1993) [4]; $E_{\text{Hicks and Comer}}$ Experimental data (Hicks and Comer, 1975) [28]; $E_{\text{Diehl et al.}}$ Experimental data (Diehl et al., 1999) [29].

doubly excited states of He-like ions up to $Z = 20$. For this state, comparison shows that MAOT results agree well with the theoretical results of [2] [4] [21] [22] [26] [27] and also the experimental data of [28] [29]. For $Z \leq 10$, comparison indicates that results agree well with each other. In addition, we calculated the energy of the ion Hydrogen H$^{-}$ where there is no available data for comparison. For $Z = 10$, our results at $-46.5156$ Ry are compared with those of [2] [4] [22] respectively at $-46.4981$ Ry; $-46.53271$ Ry and $-46.46435$ Ry. Thus, this good agreement allowed us to expect our results up to $Z = 20$ to be also accurate.

Table 3 indicates the present MAOT calculation for the $3d^1 G$ DES that are compared with those of [2] [4] [21] [30] [31]. Here, except the ion Hydrogen H$^{-}$ ($Z = 1$) where there is no available results, the agreements between the calculation are generally good up to $Z = 5$. Thus for $5 < Z \leq 10$, our results are compared with
Table 3. Parameter $\xi$ and total energies $E$ for doubly excited ($3d^2 \, ^1G$) states. The values are reported in Rydberg (Ry). $1\text{Ry} = 13.605698\text{eV}$. The screening constant sigma ($\sigma_{\text{theo}} = 0.3512$).

| Theory | $\xi$ | $E^{\text{MAOT}}$ | $E^{\text{Sakho}}$ | $E^{a}$ | $E^{b}$ | $E^{c}$ | $E^{d}$ | $E^{\text{Ray}}$ |
|--------|-------|-------------------|-------------------|--------|--------|--------|--------|-----------------|
| H$^+$  | 0.2162| 0.0152            | -                 | -      | -      | -      | -      | -               |
| He     | 0.5495| 0.6260            | 0.6104            | 0.6166 | 0.6308 | 0.6303 | 0.5849 | 0.6232         |
| Li$^+$ | 0.8829| 1.6004            | 1.5486            | 1.5538 | 1.5837 | 1.5618 | 1.5247 | 1.4601         |
| Be$^{2+}$ | 1.2162| 2.9529            | 2.9313            | 2.9762 | 2.9377 | 2.9085 | 2.8421 |                |
| B$^+$  | 1.5495| 4.7596            | 4.7585            | 4.8105 | 4.7581 | 4.7360 | 4.6669 |                |
| C$^{6+}$ | 1.8829| 7.1927            | 7.0301            | 7.0180 | 7.0875 | 7.0229 |        |                |
| Ne$^{10+}$ | 2.2162| 9.8973            | 9.7461            | 9.7280 | 9.8079 | 9.7321 |        |                |
| O$^{6+}$ | 2.5495| 13.0334           | 12.9066           | 12.882 | 12.9718| 12.8858|        |                |
| F$^{7+}$ | 2.8829| 16.5999           | 16.5116           | 16.4800| 16.5797| 16.4840|        |                |
| Ne$^{8+}$ | 3.2162| 20.5969           | 20.5609           | 20.5200| 20.6316| 20.5265|        |                |
| Na$^{9+}$ | 3.5495| 25.0246           | 25.0599           | 25.0200| 25.1316| 25.0265|        |                |
| Mg$^{10+}$ | 3.8829| 29.8814           | 29.9299           | 29.8599| 29.9800| 29.8854|        |                |
| Al$^{11+}$ | 4.2162| 35.1721           | 35.2099           | 35.1399| 35.2500| 35.1554|        |                |
| Si$^{12+}$ | 4.5495| 40.8918           | 40.9299           | 40.8599| 40.9800| 40.8854|        |                |
| P$^{13+}$ | 4.8829| 47.0424           | 47.0809           | 47.0109| 47.1316| 47.0265|        |                |
| S$^{14+}$ | 5.2162| 53.6234           | 53.6599           | 53.5899| 53.7100| 53.6154|        |                |
| Cl$^{15+}$ | 5.5495| 60.6351           | 60.6736           | 60.6051| 60.7265| 60.6216|        |                |
| Ar$^{16+}$ | 5.8829| 68.0777           | 68.1163           | 68.0463| 68.1676| 68.0725|        |                |
| K$^{17+}$ | 6.2162| 75.9507           | 76.0809           | 75.9109| 76.0316| 75.9265|        |                |
| Ca$^{18+}$ | 6.5495| 84.2544           | 84.3936           | 84.3236| 84.4451| 84.3501|        |                |

$E^{\text{MAOT}}$: Energy $E$ of the Modified Atomic Orbital Theory (MAOT), present work. $E^{\text{Sakho}}$ (Sakho, 2010) [30]; $E^a$ (Bachau et al., 1991) [31]; $E^b$ (Biaye, 2005) [2]; $E^c$ (Ivanov and Safronova, 1993) [4]; $E^d$ (Ho, 1989) as quoted in (Biaye, 2005) [2]; $E^{\text{Ray}}$ (Ray et al., 1991) [21].

those of [2] [4] [30] [31] and it can be seen that the present MAOT results agrees well with each other. Comparison indicates that ($Z = 10$) our results at −20.5969 Ry agrees very well with them respectively at −20.56099 Ry, −20.52000 Ry, −20.63354 Ry and −20.52658 Ry for [4]. In addition, the theoretical screening constant is also calculated ($\sigma_{\text{theo}} = 0.3512$). This good agreement allows us to expect our results with MAOT calculation for $3d^2 \, ^1G$ doubly excited state up to $Z = 20$ to be accurate.

In Table 4, we present our calculation for the $4f^2 \, ^1I$ doubly excited state and compare our results with theoretical results of [2] [30] and [32]. In our knowledge, experimental data are not available yet and also for the ion Hydrogen H$^+$ ($Z = 1$). Here the agreements between the calculations are seen to be very satisfactory. As far as comparisons with the SCUNC results of [2] [30] and [32] are
Table 4. Parameter $\xi$ and total energies $E$ for doubly excited $4f^1I$ states. The values are reported in Rydberg (Ry). $1\text{Ry} = 13.605698 \text{eV}$. The screening constant sigma ($\sigma_{\text{theo}} = 0.3508$).

| Theory | $\xi$ | $E_{\text{MAOT}}$ | $E_{\text{Sakho}}$ | $E_{\text{Biaye}}$ | $E_{\text{Ho}}$ |
|--------|-------|-----------------|----------------|-----------------|---------------|
| H$^+$  | 0.1623| 0.04848         |                |                 |               |
| He     | 0.4123| 0.32906         | 0.32380        | 0.3591          | 0.34080       |
| Li$^+$ | 0.6623| 0.85937         | 0.83464        | 0.89777         |               |
| Be$^{2+}$ | 0.9123| 1.65938        | 1.59547        | 1.68285         |               |
| B$^{3+}$ | 1.1623| 2.66909        | 2.60631        | 2.71550         |               |
| C$^{4+}$ | 1.4123| 3.95001        | 3.86714        | 3.99645         |               |
| N$^{5+}$ | 1.6623| 5.47766        | 5.37798        | 5.52616         |               |
| O$^{6+}$ | 1.9123| 7.25650        | 7.13881        | 7.30493         |               |
| F$^{7+}$ | 2.1623| 9.28507        | 9.14965        | 9.33300         |               |
| Ne$^{8+}$ | 2.4123| 11.56332       | 11.41048       | 11.61005        |               |
| Na$^{9+}$ | 2.6623| 14.09130       |                |                 |               |
| Mg$^{10+}$ | 2.9123| 16.86898       |                |                 |               |
| Al$^{11+}$ | 3.1623| 19.89637       |                |                 |               |
| Si$^{12+}$ | 3.4123| 23.17405       |                |                 |               |
| P$^{13+}$ | 3.6623| 26.70029       |                |                 |               |
| S$^{14+}$ | 3.9123| 30.47681       |                |                 |               |
| Cl$^{15+}$ | 4.1623| 34.50304       |                |                 |               |
| Ar$^{16+}$ | 4.4123| 38.77898       |                |                 |               |
| K$^{17+}$ | 4.6623| 43.30464       |                |                 |               |
| Ca$^{18+}$ | 4.9123| 48.07999       |                |                 |               |

$E_{\text{MAOT}}$: Energy $E$ of the Modified Atomic Orbital Theory (MAOT), present work. $E_{\text{Sakho}}$ (Sakho, 2010) [30]; $E_{\text{Biaye}}$ (Biaye et al., 2005) [2]; $E_{\text{Ho}}$ (Ho, 1989) as quoted in (Biaye et al., 2005) [2].

Concerned, our results for $Z = 2$, at $-0.32906$ Ry, agree well with them respectively at $-0.32380$ Ry; $-0.35913$ Ry and $-0.34080$ Ry. For $2 < Z \leq 10$, it can be seen the present MAOT results agrees with each other, and the agreement can be seen up to $Z = 10$ between our results at $-11.56322$ Ry and that from theoretical calculations [30] and [2] respectively at $-11.41048$ Ry, and $-11.61005$. As a result, our listed data up to $Z = 20$ are expected to be also accurate. In addition the screening constant is also calculated $\sigma_{\text{theo}} = 0.3508$. The good agreement between the results quoted in Tables 1-4 indicate the validity of this MAOT variational procedure and his merit to calculate the $(nf)$ ground-state and doubly excite state energies.

4. Summary and Conclusion

In this work, the variational procedure of the Modified Atomic Orbital Theory
MAOT has been applied for the first time to the calculations of the ground-state energy $2s^2 \, ^1S$ and excitation energies of the doubly $2p^2 \, ^1D$, $3d^2 \, ^1G$, $4f^2 \, ^1I$ excited states of the Helium isoelectronic sequence from Hydrogen ion H$^-$ to Calcium ion Ca$^{18+}$. It has demonstrated the possibilities to construct a new correlated wave function adapted to the correct description of the electron-electron correlations phenomena in the ground and in the doubly excited $nl^2$ states of the He-like systems. These very important results obtained in this work indicate the possibility to apply the MAOT variational procedure to the treatment of atomic spectra in two electron systems and probably in more complex atomic systems. The good results give also the possibility to analyze resonance energies via a very MAOT flexible procedure, in contrast to the complex procedures of experimental and theoretical methods based on the determination of the photoionization cross-section.

Acknowledgements

The authors are grateful to the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, the Orsay Institute of Molecular Sciences (OIMS), Paris, France and the Swedish International Development Agency (SIDA) for support.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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List of the Symbols

\( \sigma_{\text{theo}} \) (theo = theory): screening constant \( \sigma \) determined theoretically

\( E \): Energy

\( H \): Hamilton operator

\( N \): Normalization factor

\( T \): Kinetic Energy

\( W \): Coulombian interaction potential operator between the two electrons

\( C \): Coulombian interaction potential between the nucleus and the two electrons

\( \nabla_i \): denotes the Laplacian operator \( \nabla \) with reference to the coordinates of the vector radius \( r_i \) which detect the position of the electron \( i \).

\( \nabla_i \): is the Laplacian with reference to the coordinates of the vector radius \( r_i \) which detect the position of the electron 1.

\( \nabla_i \): Laplacian defines the coordinates of the vector radius \( r_j \) which detect the position of the electron 2.

\( r_i \): denotes the position \( r \) of the electron \( i \) relative to the nucleus

\( r_1 \) and \( r_2 \): denote respectively the position \( r \) of the electron 1 and the electron 2 relative to the nucleus.

\( |r_i - r_j| \): is an inter-electronic distance.

\( \theta, \varphi \): angular variables of the electron \( i \)

\( S \): total spin

\( h \): reduced Planck constant such as \( h = h/2\pi \) with \( h \) the Planck constant

\( N \): principal quantum number

\( l \): orbital quantum number

\( \Theta_{12} \): angle between electron 1 and electron 2.

\( \xi \): variational parameter zeta, a Greek alphabet

\( \text{H}^+ \): Hydrogen ion

\( \text{He}^2+ \): Helium atom

\( \text{Li}^+ \): Lithium ion

\( \text{Be}^{2+} \): Beryllium ion

\( \text{B}^{3+} \): Boron ion

\( \text{C}^{4+} \): Carbon ion

\( \text{N}^{5+} \): Nitrogen ion

\( \text{O}^{6+} \): Oxygen ion

\( \text{F}^{7+} \): Fluorine ion

\( \text{Ne}^{8+} \): Neon ion

\( \text{Na}^{9+} \): Sodium ion

\( \text{Mg}^{10+} \): Magnesium ion

\( \text{Al}^{11+} \): Aluminium ion

\( \text{Si}^{12+} \): Silicon ion

\( \text{P}^{13+} \): Phosphorus ion

\( \text{S}^{14+} \): Sulfur ion

\( \text{Cl}^{15+} \): Chlorine ion

\( \text{Ar}^{16+} \): Argon ion

\( \text{K}^{17+} \): Potassium ion

\( \text{Ca}^{18+} \): Calcium ion