



# The Singlet Doubly Excited $(nl)^2$ ( $n \leq 7$ ) States of He-Like Systems up to $Z=10$ and the Effect of Screen Constant ( $\alpha$ ) on the Nuclear Charge ( $Z$ )

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## To cite this article:

Abdou Diouf, Boubacar Sow, Youssou Gning, Malick Sow, Alassane Traore, Ahmadou Wague. The Singlet Doubly Excited  $(nl)^2$  ( $n \leq 7$ ) States of He-Like Systems up to  $Z=10$  and the effect of Screen Constant ( $\alpha$ ) on the Nuclear Charge ( $Z$ ). *International Journal of Applied Mathematics and Theoretical Physics*. Vol. 3, No. 4, 2017, pp. 78-85. doi: 10.11648/j.ijamtp.20170304.11

Received: June 10, 2017; Accepted: July 3, 2017; Published: August 9, 2017

**Abstract:** Calculations of the energy levels of atoms and ions with  $Z \leq 10$  are carried out in this paper using the variational method. New wave function with two terms including correlation was performed to calculate excited  $(ns^2)^1S^e$ ,  $(np^2)^1D^e$ ,  $(nd^2)^1G^e$ ,  $(nf^2)^1I^e$ ,  $(nh^2)^1M^e$  and  $(ng^2)^1K^e$  states with ( $n \leq 7$ ). The results obtained show quantitatively the great significance of electron correlation effects in the doubly excited states. These results are in compliance with some experimental and theoretical data.

**Keywords:** Energy, Wave Function, Two Terms, Excited States, Atoms and Ions

## 1. Introduction

Currently, a rapid development of studies on two-electron atomic systems is witnessed, both in the ground state and in the electron doubly excited states, also known as autoionization states [1-7]. Which are based on two electrons systems test new theoretical and experimental methods that can stretch in more complex systems later. The interest of these studies allows to better understand the phenomena of electronic correlation in the two-electron atomic systems and these studies can be used as an asset to demonstrate the importance and the influence of the phenomena of electronic correlations in the fundamental state and in the states of double electronic glow of He-like systems [3, 8-12]. On time actual several studies are focused on the counting energies of the ground state and states in two ways thrilled by some He-like systems in touch with the importance of electronic correlations. These studies use mainly the method of diagonalization [13-15], the group theory [16], the hyperspherical method [2, 17-20], the complex rotation method [21-24], and the variational method combined with the perturbation theory [5, 12]. Thus, it is very often to perform wave functions, which have already been successfully computed by a given theoretical method, are used in other theoretical methods to determine the characteristics of doubly excited states.

This is the case of the wave function proposed by Hylleraas in 1928 [25] and used by several theoretical methods [26-29]. At present, studies on the importance and the influence of electronic correlation phenomena in the ground state and in the doubly excited states of helium-like ions continue to generate considerable interest on the part of experimenters and theorists and it is in this framework that we propose a new wave function of two terms to compute the energies  $(ns^2)^1S^e$ ,  $(np^2)^1D^e$ ,  $(nd^2)^1G^e$ ,  $(nf^2)^1I^e$ ,  $(nh^2)^1M^e$  and  $(ng^2)^1K^e$  excited states of helium-like ions up to  $Z = 10$ .

## 2. Theory

The impossibility of analytically solving the corresponding Schrödinger equation:

$$H\Psi = E\Psi \quad (1)$$

comes from the term in  $r_{12} = u = |\vec{r}_1 - \vec{r}_2|$  which involves the positions of the two electrons. The exact resolution of equation (1) is then impossible without approximation because of the correlation term occurring in the expression of the total Hamiltonian  $H$ .

It is in this context that we have found a new function

$\Psi_{jkm}$  of two terms to calculate energies of the singlet doubly excited states  $(nl)^2$  of He-like systems for  $Z \leq 10$  defined by:

$$\Psi_{jkm} = \frac{1}{4\pi} \sum_{v=0}^{v=n-\ell-1} \left( n^2 r_0^2 \right)^v \left( C_{jkm} + C_{jkm} z r_{12}^m \right) e^{-\alpha(r_1+r_2)} \quad (2)$$

$$\Psi_{jkm} = \frac{1}{4\pi} \sum_{v=0}^{v=n-\ell-1} \left( n^2 r_0^2 \right)^v \left( C_{000} + C_{001} z r_{12}^m \right) e^{-\alpha(r_1+r_2)} \quad (3)$$

For  $j=k=m=0$  we have  $C_{000}=1$  and  $C_{001}$  for  $j=k=0$  and  $m=1$ . We obtain:

$$\Psi_{000} = \frac{1}{4\pi} \sum_{v=0}^{v=n-\ell-1} \left( n^2 r_0^2 \right)^v (C_{000}) e^{-\alpha(r_1+r_2)} \quad (4)$$

and

$$\Psi_{001} = \frac{1}{4\pi} \sum_{v=0}^{v=n-\ell-1} \left( n^2 r_0^2 \right)^v (C_{001} z r_{12}^m) e^{-\alpha(r_1+r_2)} \quad (5)$$

Using these expressions, equation (3) becomes

$$\Psi_{jkm} = \Psi_{000} + \Psi_{001} \quad (6)$$

$$\Psi_{jkm} = \frac{1}{4\pi} \sum_{v=0}^{v=n-\ell-1} \left( n^2 r_0^2 \right)^v (1 + C_{001} z r_{12}^m) e^{-\alpha S} \quad (7)$$

For the calculation of energies we use the formula:

$$E = \langle H \rangle = \frac{\langle \Psi_{jkm} | H | \Psi_{jkm} \rangle}{\langle \Psi_{jkm} | \Psi_{jkm} \rangle} \quad (8)$$

In Equation (8),  $H$  is the Hamiltonian defined by:

$$H = -\frac{1}{2} \Delta_1 - \frac{1}{2} \Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (9)$$

In this equation,  $Z$  is the nuclear charge  $\Delta_1$  is the Laplacian with reference to the coordinates of the vector radius  $r_1$  which detect the position of the electron 1.  $\Delta_2$  Laplacian defines the coordinates of the vector radius  $r_2$  which detect the position of the electron 2 and  $r_{12}$  inter- electronic distance.

Volume integrals can be written as follows:

$$\int d\tau = 8\pi^2 \int r_1^2 r_2^2 dr_1 dr_2 \sin \theta_{12} d\theta_{12} \quad (10)$$

They know that:

$$\iint dr_1^3 dr_2^3 \left| \vec{r}_1, \vec{r}_2 \right\rangle \left\langle \vec{r}_1, \vec{r}_2 \right| = 1 \quad (11)$$

Using this relationship, we derive from the mean value of equation (8)

$$E \iint dr_1^3 dr_2^3 \left\langle \Psi_{jkm} \left| \vec{r}_1, \vec{r}_2 \right\rangle \left\langle \vec{r}_1, \vec{r}_2 \right| \Psi_{jkm} \right\rangle = \iint dr_1^3 dr_2^3 \left\langle \Psi_{jkm} \left| \vec{r}_1, \vec{r}_2 \right\rangle \hat{H} \left\langle \vec{r}_1, \vec{r}_2 \right| \Psi_{jkm} \right\rangle \quad (12)$$

By expanding this expression we obtain:

$$E \iint dr_1^3 dr_2^3 \Psi_{jkm} ? \Psi_{jkm}^* = \iint dr_1^3 dr_2^3 \Psi_{jkm} \hat{H} \Psi_{jkm}^* \quad (13)$$

Namely:

$$N * E = \iint dr_1^3 dr_2^3 \Psi_{jkm} \hat{H} \Psi_{jkm}^* \quad (14)$$

With

$$N = \iint dr_1^3 dr_2^3 \left| \Psi_{jkm} \right|^2 \quad (15)$$

The normalization constant and the elementary volume element

$$d\tau = dr_1^3 dr_2^3 \quad (16)$$

To facilitate the integration of the equation, one transforms the polar into elliptical coordinates and asked [31]:

$$\begin{cases} \text{for } \theta_{12} = \pi, & u = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}} = \sqrt{r_1^2 + r_2^2 + 2r_1 r_2} = \sqrt{(r_1 + r_2)^2} = r_1 + r_2 \\ \text{for } \theta_{12} = 0, & u = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12}} = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2} = \sqrt{(r_1 - r_2)^2} = |r_1 - r_2| \end{cases} \quad (20)$$

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

With

$$u^2 = r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12} \quad (17)$$

and this equation gives

$$udu = r_1 r_2 \sin \theta_{12} d\theta_{12} \quad (18)$$

Equation (10) becomes

$$\int d\tau = 8\pi^2 \int_0^\infty \int_0^\infty r_1 r_2 dr_1 dr_2 \int_{|r_1 - r_2|}^{r_1 + r_2} u du \quad (19)$$

and this equation appears in the work of Hylleraas [30]  
With

Also

$$r_1 r_2 = \frac{1}{4}(s^2 - t^2) \quad (21)$$

$$\int d\tau = 2\pi^2 \int_0^\infty ds \int_0^S dt \int_t^S (s^2 - t^2) u du \quad (23)$$

and this equation becomes

$$d\tau=2\pi^2(s^2-t^2)u\,ds\,dt\,du \quad (24)$$

and this equation becomes

$$dr_1 dr_2 = \frac{1}{2} ds dt \quad (22)$$

Equation (15) and (13) respectively

$$N = \int_0^\infty ds \int_0^s du \int_0^u dt (s^2 - t^2) \times \Psi_{jkm}^2 \quad (25)$$

Finally we obtain (for an infinite volume):

$$N * E = \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[ \left( \frac{\partial \Psi^{jkm}}{\partial s} \right)^2 + \left( \frac{\partial \Psi^{jkm}}{\partial t} \right)^2 + \left( \frac{\partial \Psi^{jkm}}{\partial u} \right)^2 \right] + \right. \\ \left. 2 \left( \frac{\partial \Psi^{jkm}}{\partial u} \right) \times \left[ s(u^2 - t^2) \frac{\partial \Psi^{jkm}}{\partial s} + t(s^2 - u^2) \frac{\partial \Psi^{jkm}}{\partial t} \right] - \Psi_{jkm}^2 [4Zsu - s^2 + t^2] \right\} \quad (26)$$

$$2\left(\frac{\partial \Psi^{jkm}}{\partial u}\right) \times \left[ s(u^2 - t^2) \frac{\partial \Psi^{jkm}}{\partial s} + t(s^2 - u^2) \frac{\partial \Psi^{jkm}}{\partial t} \right] - \Psi_{jkm}^2 \left[ 4Zsu - s^2 + t^2 \right] \Bigg\}$$

$|\psi_{jkm}\rangle$  is expressed as a linear combination of respect to the parameters  $c_i$ . Namely approximate base vectors, either

$$|\psi_{jkm}\rangle = \sum_{i=1}^n c_{ijk} |\phi_{ijk}\rangle \quad (27)$$

and putting

$$|\phi_{jkm}\rangle = |\phi_i\rangle \quad (28)$$

Let us then put equation (8)

$$\langle H \rangle = \frac{\sum_{i=1}^n \sum_{j=1}^n c_i c_j \langle \phi_i | H | \phi_j \rangle}{\sum_{i=1}^q \sum_{j=1}^{q'} c_i c_j \delta_{ij}} = \frac{\sum_{i=1}^n c_i^2 \langle \phi_i | H | \phi_j \rangle}{\sum_{i=1}^n c_i^2} \quad (29)$$

with  $c_j = C_{000} = C_{001}$

The parameters  $c_i$  are determined by calculating the average value  $\langle H \rangle$  and by minimizing this value with

### 3. Results and Discussions

The obtained results for total energies, total electron-electron interaction energies and excitation energies are displayed in Tables 1-5 and the comparison tables 6-10. The results of our energy calculations singlet doubly excited states, obtained using equation (8) for  $(ns^2)^1S^e$ ,  $(np^2)^1D^e$ ,  $(nd^2)^1G^e$ ,  $(nf^2)^1I^e$ ,  $(nh^2)^1M^e$  and  $(ng^2)^1K^e$  with  $n \leq 7$  of He-like ions up to  $Z=10$ .

By fixing:  $C_{000}=0.25$  and  $\alpha=0.24$  and we calculate the parameters  $C_{001}$  of the equation (30). For comparison with the other theoretical results, we use for energy conversion: 1a.u. = 27.211396 eV and 1Ryd = 13.605698 eV.

**Table 1.** Energy doubly excited ( $ns^2$ )  $^1S^e$  ( $n \leq 7$ ) states of He-like systems up to  $Z = 10$ . The energies are in eV.

[illegible]

States	Z	2	3	4	5	6	7	8	9	10
$7s^2\ ^1S^e$	$\alpha$	0.065	0.102	0.140	0.177	0.214	0.250	0.287	0.325	0.362
	-E	2.328	5.738	10.739	17.197	25.168	34.514	45.491	58.161	72.184
	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.048	0.076	0.102	0.130	0.157	0.184	0.211	0.238	0.265
	-E	1.720	4.276	7.824	12.630	18.463	25.399	33.440	42.585	52.833

**Table 2.** Energy doubly excited  $(np^2)\ ^1D^e$  ( $n \leq 7$ ) states of He-like systems up to  $Z = 10$ . The energies are in eV.

States	Z	2	3	4	5	6	7	8	9	10
$2p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.175	0.108
	$\alpha$	0.565	0.910	1.250	1.640	2.030	2.480	3.200	3.500	3.500
	-E	19.106	48.347	90.234	147.941	217.305	300.126	397.233	508.376	632.721
$3p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.240	0.390	0.530	0.680	0.830	0.980	1.130	1.280	1.430
	-E	8.503	21.739	40.322	65.527	96.778	134.032	177.224	177.224	281.051
$4p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.135	0.220	0.300	0.380	0.460	0.550	0.630	0.714	0.795
	-E	4.821	12.351	22.974	36.868	54.031	75.832	99.727	127.589	158.270
$5p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.086	0.140	0.190	0.240	0.290	0.350	0.400	0.455	0.510
	-E	3.078	7.873	14.571	23.314	34.103	48.316	63.398	81.419	101.687
$6p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.061	0.097	0.133	0.170	0.207	0.244	0.281	0.318	0.355
	-E	2.185	5.457	10.202	16.517	24.345	33.686	44.540	56.907	70.788
$7p^2\ ^1D^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.043	0.071	0.098	0.125	0.152	0.179	0.207	0.230	0.261
	-E	1.541	3.995	7.518	12.144	17.875	24.709	32.806	41.152	52.035

**Table 3.** Energy doubly excited  $(nd^2)\ ^1G^e$  ( $n \leq 7$ ) states of He-like systems up to  $Z = 10$ . The energies are in eV.

States	Z	2	3	4	5	6	7	8	9	10
$3d^2\ ^1G^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.240	0.390	0.540	0.680	0.830	0.980	1.140	1.290	1.440
	-E	8.503	21.739	41.067	65.527	96.778	134.032	178.740	227.965	282.921
$4d^2\ ^1G^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.150	0.220	0.300	0.390	0.470	0.550	0.640	0.720	0.800
	-E	5.351	12.351	22.974	37.833	55.200	75.832	101.301	128.654	159.258
$5d^2\ ^1G^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.085	0.135	0.190	0.243	0.296	0.350	0.403	0.456	0.510
	-E	3.042	7.592	14.571	23.605	34.808	48.316	63.873	81.598	101.687
$6d^2\ ^1G^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.057	0.095	0.132	0.250	0.285	0.321	0.358	0.394	0.431
	-E	2.042	5.345	10.126	24.284	33.515	44.315	56.745	70.509	85.944
$7d^2\ ^1G^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.042	0.070	0.097	0.124	0.152	0.178	0.206	0.233	0.260
	-E	1.505	3.939	7.441	12.047	17.875	24.571	32.647	41.689	51.835

**Table 4.** Energy doubly excited  $(nf^2)\ ^1F^e$  ( $n \leq 7$ ) states of He-like systems up to  $Z = 10$ . The energies are in eV.

States	Z	2	3	4	5	6	7	8	9	10
$4f^2\ ^1F^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.141	0.216	0.306	0.387	0.470	0.554	0.637	0.720	0.800
	-E	5.033	12.127	23.431	37.544	55.209	76.381	100.828	128.654	159.258
$5f^2\ ^1F^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.082	0.135	0.188	0.242	0.295	0.349	0.401	0.455	0.503
	-E	2.935	7.592	14.418	23.508	34.691	48.178	63.557	81.419	100.293
$6f^2\ ^1F^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.058	0.094	0.131	0.167	0.205	0.242	0.279	0.316	0.353
	-E	2.077	5.289	10.049	16.225	24.109	33.410	44.223	56.549	70.389
$7f^2\ ^1F^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.042	0.069	0.096	0.123	0.151	0.178	0.205	0.232	0.259
	-E	1.505	3.882	7.364	11.950	17.757	24.571	32.489	41.511	51.636

**Table 5.** Energy doubly excited  $(ng^2)^1K^e$ ,  $(nh^2)^1M^e$  ( $n \leq 7$ ) states of He-like systems up to  $Z = 10$ . The energies are in eV.

States	Z	2	3	4	5	6	7	8	9	10
$5g^2^1K^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.082	0.135	0.188	0.241	0.295	0.347	0.402	0.454	0.508
	-E	2.935	7.592	14.418	23.411	34.691	47.902	63.715	81.241	101.289
$6g^2^1K^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.057	0.093	0.131	0.167	0.205	0.242	0.279	0.316	0.353
	-E	2.042	5.232	10.049	16.225	24.109	33.410	44.223	56.549	70.389
$7g^2^1K^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.042	0.069	0.096	0.123	0.151	0.177	0.205	0.232	0.259
	-E	1.505	3.882	7.364	11.950	17.757	24.433	32.489	41.511	51.636
$6h^2^1M^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.057	0.093	0.130	0.167	0.205	0.241	0.278	0.315	0.352
	-E	2.042	5.232	9.972	16.225	24.109	33.272	44.064	56.371	70.189
$7h^2^1M^e$	$C_{001}$	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250	0.250
	$\alpha$	0.041	0.068	0.096	0.123	0.150	0.177	0.204	0.232	0.259
	-E	1.469	3.826	7.364	11.950	17.639	24.433	32.330	41.511	51.636

In the Table 6 our results are compared with those obtained by Gning [27] using a complex rotation method implemented in Scilab, Sakho [31] using the screening constant by unit nuclear charge method, Ho [32] using the complex-coordinate rotation method. Besides, for theoretical results, a good agreement is observed comparing our total energies for  $(ns^2)^1S^e$ ,  $n \leq 7$  to those of the available. We note a small disagreement between our results and the other theoretical calculations. These disagreements can be explained by the choice of the wave functions for the 3s, 4s and 5s  $^1S^e$  states the comparison with the theoretical values of Gning, Ho gives a good agreement.

In Table 7, we compare our results with those of Ivanov [33] using double sum method over the complete hydrogen spectrum, A. K. Roy [34] using density functional-theory results, S. Diehl [35]. With available experimental result of  $Li^+$  obtained and for also doubly excited states we see excellent agreement between our values and those of Sakho

[31] for the  $(np^2)^1D^e$  state. For these states, we note generally a quite good agreement between our results and those of Sakho, Ivanov and Roy for low values.

In Table 8 As regards the  $(nd^2)^1G^e$  levels, comparison shows also a good agreement with variational Hylleraas results of Biaye [36] density functional-theory results of Roy et al. [34] and time-dependant perturbation theory results of Ray and Mukherjee [37]. A very good agreement is also noted between our results and that of Diehl [35]. We find generally a satisfactory agreement between the present calculations with  $Z \leq 7$  and those of Biaye.

Table 9 compares our results with the theoretical results of Sakho [31] and Biaye [36] for the  $(nf^2)^1I^e$  state. We note generally a satisfactory agreement between our results and those of Sakho and Biaye.

We compare our results in Table 10 with those of Sakho [31] for the  $(ng^2)^1K^e$  and  $(nh^2)^1M^e$  state. We note generally a good agreement between our results with those of Sakho.

**Table 6.** A Comparison of the doubly excited  $(ns^2)^1S^e$  states with He-like systems up to  $Z = 10$  with other results. The energies are in eV.

States $ns^2^1S^e$	Z	2	3	4	5	6	7	8	9	10
$2s^2^1S^e$	-E <sup>p</sup>	21.09	51.00	95.94	153.74	226.90	312.00	408.60	520.43	646.92
	E <sup>a</sup>	21.16	51.86	96.15	154.03	225.53	310.62	409.33	521.62	647.54
	E <sup>b</sup>	21.19	52.00	96.43	154.45	226.09	311.32	410.17	522.62	648.67
	E <sup>c</sup>	21.16	51.86	96.15	154.04	225.53	310.63	409.33	521.62	647.54
$3s^2^1S^e$	-E <sup>p</sup>	9.64	23.37	43.29	69.28	100.18	138.41	181.76	231.35	286.65
	E <sup>a</sup>	9.61	23.40	43.23	69.10	101.02	138.98	182.99	233.05	289.15
	E <sup>b</sup>	9.42	23.11	42.86	68.65	100.48	138.37	182.30	232.27	288.30
	E <sup>c</sup>	9.61	23.40	43.22	69.10	101.02	138.98	182.99	233.05	289.15
$4s^2^1S^e$	-E <sup>p</sup>	5.35	13.18	24.49	38.08	57.95	78.43	103.18	130.42	163.20
	E <sup>b</sup>	5.30	13.00	24.11	38.61	56.52	77.83	102.54	130.65	162.17
$5s^2^1S^e$	-E <sup>p</sup>	3.22	8.15	15.33	24.28	36.45	49.69	65.29	83.20	103.67
	E <sup>b</sup>	3.39	8.32	15.43	24.71	36.17	49.81	65.63	83.62	103.79
$6s^2^1S^e$	-E <sup>p</sup>	2.35	5.78	10.71	17.16	25.12	34.59	45.57	58.07	72.07
	E <sup>b</sup>	2.35	5.78	10.71	17.16	25.12	34.59	45.57	58.07	72.07
$7s^2^1S^e$	-E <sup>p</sup>	1.72	4.27	7.82	12.63	18.46	25.39	33.44	42.58	52.83
	E <sup>b</sup>	1.73	4.24	7.87	12.61	18.46	25.41	33.48	42.66	52.95

<sup>p</sup> Present work, <sup>a</sup> Gning [27], <sup>b</sup> Sakho [31], <sup>c</sup> Ho [32]

**Table 7.** A Comparison of the doubly excited  $(np^2)^1D^e$  states with He-like systems up to  $Z = 10$  with other results. The energies are in eV.

States $np^2^1D^e$	Z	2	3	4	5	6	7	8	9	10
$2p^2^1D^e$	-E <sup>p</sup>	19.10	48.34	90.23	147.94	217.30	300.12	397.23	508.37	632.72
	E <sup>a</sup>	19.4	48.39	90.97	147.16	216.95	300.35	397.35	507.97	632.18
	E <sup>b</sup>		47.77	90.54	146.91					
	E <sup>c</sup>		48.18	90.82	147.04					

States $np^2 1D^e$	Z	2	3	4	5	6	7	8	9	10
$3p^2 1D^e$	$E^d$	19.12	48.73	91.95	148.77	219.20	303.24	400.88	512.13	636.98
	$-E^p$	8.50	21.73	40.32	65.52	96.77	134.03	177.22	177.22	281.05
	$E^a$	8.99	22.11	41.28	66.50	97.76	135.07	178.43	227.83	283.29
	$E^b$		21.83	41.09	66.41					
$4p^2 1D^e$	$E^c$		21.67	40.79	65.94					
	$E^d$	8.50	21.66	40.87	66.12	97.42	134.77	178.17	227.61	283.10
	$-E^p$	4.82	12.35	22.97	36.86	54.03	75.83	99.72	127.58	158.27
	$E^b$		12.38	23.26	37.54					
$5p^2 1D^e$	$E^d$	4.78	12.18	22.99	37.19	54.80	75.81	100.22	128.03	159.24
	$-E^p$	3.07	7.87	14.57	23.31	34.10	48.31	63.39	81.41	101.68
	$E^b$		7.95	14.93	24.08					
	$E^d$	3.06	7.80	14.71	23.80	35.07	48.52	64.14	81.94	101.92
$6p^2 1D^e$	$-E^p$	2.18	5.45	10.20	16.51	24.34	33.68	44.54	44.54	70.78
	$E^d$	2.12	5.41	10.22	16.53	24.36	33.69	44.54	56.90	70.77
	$-E^p$	1.54	3.99	7.51	12.63	17.87	24.70	32.80	41.15	52.03
	$E^d$	1.56	3.98	7.51	12.14	17.89	24.75	32.72	41.81	52.00

<sup>p</sup> Present work, <sup>a</sup> Ivanov [33], <sup>b</sup> Roy [34], <sup>c</sup> Diehl [35], <sup>d</sup> Sakho [31]

**Table 8.** A Comparison of the doubly excited  $(nd^2) 1G^e$  states with He-like systems up to  $Z = 10$  with other results. The energies are in eV.

States $nd^2 1G^e$	Z	2	3	4	5	6	7	8	9	10
$3d^2 1G^e$	$-E^p$	8.50	21.73	41.06	65.52	96.77	134.03	178.74	227.96	282.92
	$E^a$	8.58	8.58	40.49	65.46	96.44	133.46	133.46	225.60	280.73
	$E^b$	7.96	20.74	39.57	64.44					
	$E^c$	8.49	21.15	39.84	64.56					
$4d^2 1G^e$	$E^d$	8.35								
	$-E^p$	5.35	12.35	22.97	37.83	55.20	75.83	101.30	128.65	159.25
	$E^a$	4.89	12.24	22.94	37.02	54.50	75.36	99.63	127.31	158.38
	$E^b$	4.70	12.06	22.82	36.98					
$5d^2 1G^e$	$E^c$	5.31	12.52	23.33	37.55					
	$-E^p$	3.04	7.59	14.57	23.60	34.80	48.31	63.87	81.59	101.68
	$E^b$	3.07	7.81	14.74	23.84					
	$-E^p$	2.04	5.34	10.12	24.28	33.51	44.31	56.74	70.50	85.94
$6d^2 1G^e$	$E^b$	2.15	5.46	10.28	16.61					
	$-E^p$	1.50	3.93	7.44	12.04	17.87	24.57	32.64	41.68	51.83
	$E^b$	1.59	4.02	7.57	12.23					

<sup>p</sup> Present work, <sup>a</sup> Biaye [36], <sup>b</sup> Roy [34], <sup>c</sup> Ray [37], <sup>d</sup> Diehl [35]

**Table 9.** A Comparison of the doubly excited  $(nf^2) 1F^e$  states with He-like systems up to  $Z = 10$  with other results. The energies are in eV.

States $nf^2 1F^e$	Z	2	3	4	5	6	7	8	9	10
$4f^2 1F^e$	$-E^p$	5.03	12.12	23.43	37.54	55.20	76.38	100.82	128.65	159.25
	$E^a$	4.62	11.92	22.63	36.74	54.25	75.16	99.47	127.18	158.30
	$E^c$	4.89	12.22	22.90	36.95	54.38	75.19	99.40	126.99	157.98
	$-E^p$	2.93	7.59	14.41	23.50	34.69	48.17	63.55	81.41	100.29
$5f^2 1F^e$	$E^a$	2.95	7.63	14.48	23.51	34.72	48.10	63.66	81.40	101.31
	$-E^p$	2.07	5.28	10.04	16.22	24.10	33.41	44.22	56.54	70.38
	$E^a$	2.05	5.30	10.06	26.33	24.11	33.40	44.21	56.53	70.35
	$-E^p$	1.50	3.88	7.36	11.95	17.75	24.57	32.48	41.51	51.63
$7f^2 1F^e$	$E^a$	1.51	3.89	7.39	11.99	17.71	24.54	32.48	41.53	51.69

<sup>p</sup> Present work, <sup>a</sup> Sakho [31], <sup>c</sup> Biaye [36].

**Table 10.** A Comparison of the doubly excited  $(ng^2) 1K^e$  and  $(nh^2) 1M^e$  states with He-like systems up to  $Z = 10$  with other results. The energies are in eV.

States $ng^2 1K^e$ $nh^2 1M^e$	Z	2	3	4	5	6	7	8	9	10
$5g^2 1K^e$	$-E^p$	2.93	7.59	14.41	23.41	34.69	47.90	63.71	81.24	101.28
	$E^a$	2.93	7.59	14.42	23.44	34.63	47.99	63.54	81.26	101.16
	$-E^p$	2.04	5.23	10.04	16.22	24.10	33.41	44.22	56.54	70.38
	$E^a$	2.03	5.27	10.02	16.27	24.05	33.33	44.12	56.43	70.25
$7g^2 1K^e$	$E^a$	1.50	3.88	7.36	11.95	17.75	24.43	32.48	41.51	51.63
	$E^a$	1.49	3.87	7.36	11.96	17.67	24.49	32.42	41.46	51.61
	$-E^p$	2.04	5.23	9.97	16.22	24.10	33.27	44.06	56.37	70.18
	$E^a$	2.02	5.25	9.99	16.24	24.01	33.28	44.07	56.37	70.18
$7h^2 1M^e$	$-E^p$	1.46	3.82	7.36	11.95	17.63	24.43	32.33	41.51	51.63
	$E^a$	1.48	3.86	7.34	11.93	17.64	24.45	32.38	41.42	51.56

<sup>p</sup> Present work, <sup>a</sup> Sakho [31].

The curves of Figures 1-4 compare our results on the values of the screen constants  $\alpha$  as a function of  $Z$  of the 2s, 3s, 2p, 3p, 3d, 4d and 4f states of the doubly excited singlet states with those obtained by Sow [38], using a new wave function to four-term. We can notice the good agreement that it has in general on the increase of the screen constant  $\alpha$  when  $Z$  increases for the two-term wave function. In the case of the four-term wave function, we see that for each state almost  $\alpha$  is a constant and this can be explained by the choice, ie the position of  $\alpha$  in the wave function. And it is well known that the electron becomes increasingly tied as  $Z$  increases as the electric charge of the nucleus increases with  $Z$ , which increases the attraction of the electrons, causing the increase of  $\alpha$  as a function of  $Z$ . These are clearly observed with the use of the two-term wave function.

The energies of doubly excited singlet states of He-like ions are included in the classification of multiplets (series of lines) for electrons of the same valence. This classification reveals an important aspect of electronic correlations. The spacing of the energy levels of the multiplets of the atomic states of the same valence is identical the rotation spectra of the triatomic linear molecules. Because in the doubly excited states of weak nuclear charge  $Z$  the electron-electron interactions are of the same order of magnitude as the electron-nucleus interactions and The two electrons always have a strong tendency to oppose one to side of the nucleus [39-41] and these results in a linear distribution of the electronic charge density in a linear molecule.

This resemblance disappears as the nuclear charge  $Z$  increases due to the fact that electron-electron interactions become increasingly negligible in the face of electron-core interaction. These aspects of the spacing energies are in good agreement with the results obtained in Figures 1-4 for a new to two-term. It is for the first time to our knowledge that we have used a wave function of two terms for the calculation of the energies of doubly excited singlet states. Similarly screen constant that are compared as a function of terms used in wave functions of two and four terms used by Sow [38]. The reading of the results grouped in Figures 1-4 shows that the use of wave functions of two terms clearly explains the variations of screen constant as a function of  $Z$  is more precise than that of a wave function of four terms.

## 4. Conclusion

It has demonstrated the possibilities to use a new wave function in the study of  $(ns^2)^1S^e$ ,  $(np^2)^1D^e$ ,  $(nd^2)^1G^e$ ,  $(nf^2)^1I^e$ ,  $(nh^2)^1M^e$  and  $(ng^2)^1K^e$  doubly excited states in the helium-like ions in the framework of a variational procedure.

The interest of these studies is to understand better the phenomena of electronic correlations in two-electron atomic systems. These systems by which new experimental and theoretical methods can be tested which can then extend to more complex systems. These studies highlight the importance and influence of electronic correlation phenomena in the ground state and in the doubly excited

states of He-like ions. These very important results also make it possible to analyze resonance energies via a very flexible procedure, in contrast to the complex procedures of experimental and theoretical methods based on the determination of the photoionization cross-section.

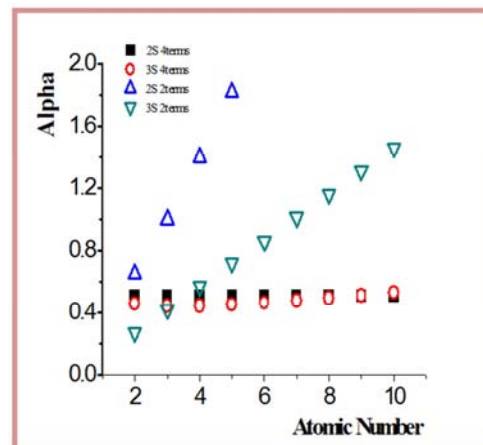


Figure 1. Comparison of the screen constant ( $\alpha$ ) as a function of  $Z$  of  $ns^2$  of the wave functions of 2 and 4 terms.

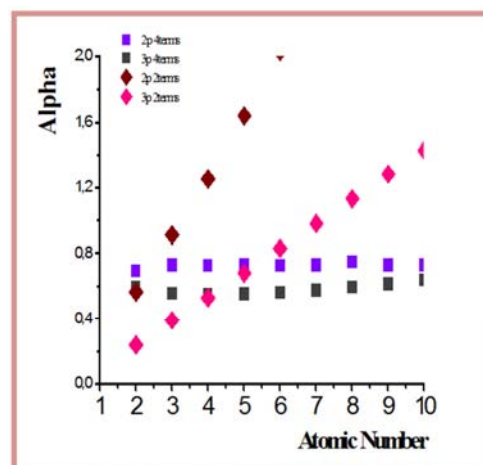


Figure 2. Comparison of the screen constant ( $\alpha$ ) as a function of  $Z$  of  $np^2$  of the wave functions of 2 and 4 terms.

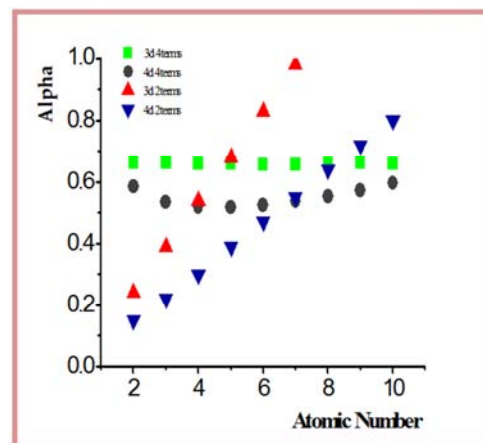
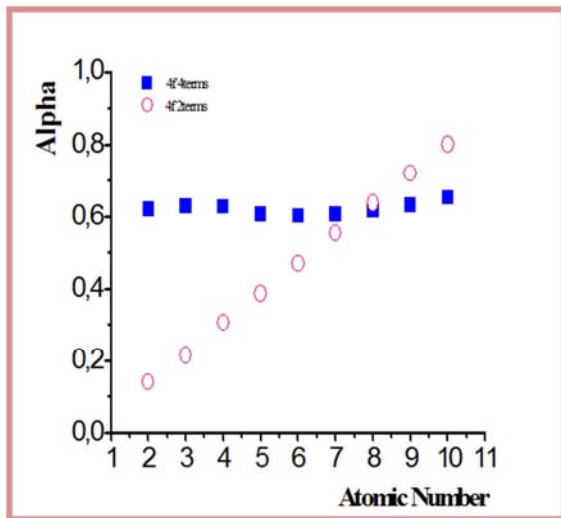


Figure 3. Comparison of the screen constant ( $\alpha$ ) as a function of  $Z$  of  $nd^2$  of the wave functions of 2 and 4 terms.



**Figure 4.** Comparison of the screen constant ( $\alpha$ ) as a function of  $Z$  of  $nf^2$  of the wave functions of 2 and 4 terms.

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