Calculations of $2s^{n+1,3}S^e$, $2snp^{+1,3}P^0$, $2pnp^{+1,3}D^e$
Autoionizing States in Two-Electrons Systems Using a New Wave Function to Four Terms

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Abstract: In this paper, we calculate energies for $2s^{n+1,3}S^e$, $2snp^{+1,3}P^0$, $2pnp^{+1,3}D^e$ autoionizing states of helium-like ions. These calculations are investigated using a new wave function correlated to four terms. Total energies calculations are performed between two electrons in He-isoelectronic series up to $Z = 10$, based on the Screening Constant by Unit Nuclear charge method in the framework of a variational procedure. The results obtained are in compliance with recent theoretical calculations.

Keywords: Autoionizing States, Wave Function Correlated, He-Isoelectronic, Screen Constant by Unit Nuclear Charge

1. Introduction

Currently in atomic physics the studies concerning the determination of the characteristics of the doubly excited states such as total energies, the total widths as well as the cross sections of autoionisation are of a great importance. These studies allowed the theorists and the experimenters to highlight the importance of the phenomena of electronic correlation in the doubly excited states of the atomic systems with two electrons. [1-6].

Many efforts were deployed in the last few years in the clarification of several theoretical methods for the description of the atomic systems with two electrons; it is still possible to make other studies in this field in order to test new theoretical methods which can contribute to a better understanding of the phenomena of electronic correlations. Within this framework that a new wave function of four special terms of Hylleraas forms type was developed to describe the atomic systems with two doubly excited He atom and He-like ions with $Z \leq 15$ [7-8].

These kinds of wave functions of special shape are used for the calculation of energy to the ground state and use more terms [9-11]. They allowed also with the use of the variational method combined with the theory of the interaction of the configurations, to describe in a very satisfactory way some singlets states of the same valence (nl$^2$, nlnl$^1$ with $n \leq 4$) doubly excited of helium and He atom and He-like ions with [12−15].

This work constitutes a generalization of the studies to several doubly excited singulets and triplets $2s^{n+1,3}S^e$, $2snp^{+1,3}P^0$ and $2pnp^{+1,3}D^e$ states of the same electrons valence by using a new wave function of special forms of hylleraas types to four terms.

2. Theory

The calculation of the energy of the fundamental state was an outstanding contribution for quantum mechanics. A method of calculating energies of the fundamental state of helium and the space part associated with the function of wave was proposed by Hylleraas in 1928. [16]

The Hylleraas method was applied successfully by himself in the calculation of the energy of the fundamental state of He atom and He-like ions. To expand this application to calculate the total energy of atomic systems in the doubly excited states
must seek new wave functions correlated \( \psi(\vec{r}_1, \vec{r}_2) \) adapted to the description of those states.

The helium atom and its isoelectronic series are atomic systems with two electrons. By neglecting the relativistic effects (variation of the mass of the electrons with speed, interaction spin-spin, spin-orbit coupling) and magnetic effects (had with the electric currents generated by the orbital movements of the electrons), Hamiltonian associated with the two electrons (1) and (2) with He atom and He-like ions is written in the approximation of the infinitely heavy core (what supposes the motionless core):

\[
H = -\frac{1}{2}[\Delta_1 - \frac{1}{2}\Lambda_2] - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{\eta_12}
\]  

in a.u. 

(1)

This equation can be put in the form:

\[
H = H_1 + H_2 + W
\]

(2)

In the equation (2), \( H \) and \( W \) respectively indicate the no disturbed Hamiltonian and it is given by the following relations:

\[
H_1 + H_2 = -\frac{1}{2}[\Delta_1 - \frac{1}{2}\Lambda_2] - \frac{Z}{r_1} - \frac{Z}{r_2}
\]

(3)

and

\[
W = \frac{1}{\eta_12}
\]

(4)

In these equations: \( Z \) 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 \( \eta_{12} = |r_1 - r_2| \) inter-electronic distance. Moreover, the Schrödinger equation applied to He-like systems is then written:

\[
\hat{H}\psi = E\psi
\]

(5)

The existence of the term of disturbance (4) then makes impossible the exact resolution of the equation (5).

It is thus we used the variational method which is one of the techniques of calculation making it possible to provide approximate solutions to the resolution of the equation of Schrödinger applied to the atomic systems with two electrons.

It is for this reason one is brought to implement an approximate method of calculating using a function of wave known as correlated \( \Psi \) of four terms which is given by:

\[
\Psi(r_1, r_2, \alpha) = k P(r_1, r_2, \alpha)e^{-4(\eta_1 + \eta_2)}
\]

(6)

with

\[
P(r_1, r_2, \alpha) = c_1 + c_2 (r_1 + r_2)(\eta_{12})^2 + c_3 (\eta_1 - \eta_2) + z\alpha \eta_{12}
\]

(7)

\[
k = \left( \frac{\sqrt{2}}{2} \right)^{n+\ell+3/2+2(n)l}
\]

(8)

\( C_1, C_2, C_3 \) are fixed parameters for the ground state and in the excited state and the Screening Constant \( \alpha \) reflecting the effect exerted by the charges of the electrons on the nuclear charge. \( Z \) the nuclear charge.

The normalization constant.

\[
N = \iint \, dt \, \, dr \, dr \, \left| \psi(r_1, r_2, \alpha) \right|^2
\]

(9)

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

\[
s = (r_1 + r_2); \ t = (r_1 - r_2); \ u = \eta_{12} \]

Based on these variable changes, the elementary volume element

\[
d\tau = d\eta_1^3 d\eta_2^3
\]

is written:

\[
d\tau = 2\pi^2 (s^2 - t^2) \, ds \, dt \, du
\]

(10)

The normalization constant and correlated wave function are reduced to the simple form:

\[
N = \int_0^u \int_0^u \int_0^u \left\{ (s^2 - t^2) \right\} x \Psi^2
\]

(11)

\[
\Psi(s,t,u) = \left( \frac{\sqrt{2}}{2} \right)^{n+\ell+3/2+2(n)l} \left\{ (c_1 + c_2 s t^2 + c_2 t + z\alpha) e^{-4s} \right\}
\]

(12)

General expressions of total energies \( 2s3s^+) \), \( 2s4s^+) \), \( 2snp^+) \), \( 2p3p^+) \), \( 2p4p^+) \) singlets and triplets excited states of He-like ions.

To pass to the eigenvalues, equation (2) gives for the ground state

\[
E(1S_0) = E_1^{(0)} + E_1^{(2)} + W_1
\]

Using the perturbation theory, one finds for the average value of the electron correlation term (2) to the first-order approximation [18].

\[
W_1 = \frac{5}{4} Z E_{II}
\]

With

\[
E_{II} = \frac{1}{2} \alpha^2 \mu_0 e^2
\]

(13)

(14)

(15)

(16)

(17)

(18)

Let us rewrite the result (15) that provides the perturbation theory to the first-order approximation as follows:
Let us then put
\[
\varepsilon_1 = \left( \frac{5}{4Z} \right)
\]  
(18)

By use of equation (17), (18) can be written in the form
\[
E(1S_0) = E^{(1)}_1 + E^{(2)}_1 + \varepsilon_1 Z^2 E_H = \varepsilon_1 Z^2 E_H
\]  
(19)

For convenience of language, we will call \(\varepsilon_1\) the perturbation coefficient taking into account the electron correlation to the first approximation. Using (14) and (19), let us write the value of the ground-state energy to the \(p\) orders of various approximation as follows:

\[
(1) \quad (2) \quad 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 1 \quad 1
\]
\[
(1) \quad (2) \quad 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 1 \quad 1
\]
\[
E^{(1)}_1 + E^{(2)}_1 + \varepsilon_1 Z^2 + \varepsilon_2 Z^4 + \varepsilon_3 Z^6 + \varepsilon_4 Z^8 + L + L \varepsilon_p Z^2 E_H
\]  
(20)

That means
\[
E(1S_0) = E^{(1)}_1 + E^{(2)}_1 + (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + L + L \varepsilon_p + O(\varepsilon_v)) Z^2 E_H
\]  
(21)

To a \(q\)-order approximation as elevated as possible, let us write (21) in the form
\[
E(1S_0) = E^{(1)}_1 + E^{(2)}_1 + \left( \sum_{p=1}^{q} \varepsilon_p \right) Z^2 E_H
\]  
(22)

Otherwise, taking into account the fact that,
\[
E^{(1)}_1 = E^{(2)}_1 = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2
\]  
(23)

equation (22) becomes
\[
E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 + \left( \sum_{p=1}^{q} \varepsilon_p \right) Z^2 E_H
\]  
(24)

Using (16), one gets from (23)
\[
E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 + \left( \sum_{p=1}^{q} \varepsilon_p \right) Z^2 \alpha^2 m_0 c^2
\]  
(25)

Let us arrange then (25) as follows
\[
E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 + \left( \sum_{p=1}^{q} \varepsilon_p \right) Z^2 \alpha^2 m_0 c^2
\]  
(26)

As expressed, the second term of the right-hand side of equation (26) corresponds to the interaction energy of an electron-hydrogenic atom system of effective charge \(Z^\ast\) defined by
\[
Z^\ast = Z \left[ 1 - \beta(1S_0, Z) \right]^{\frac{1}{2}}
\]  
(27)

As defined by (31), the \(\beta(1S_0, Z)\)-parameter plays the role of the screening constant assumed to depend on the charge number \(Z\) and the number of electrons of the considered atomic system (two electrons in the case of helium isoelectronic sequence).

The result (31) gives the expression of the effective nuclear charge \(Z^\ast\) to the ground state. This result is generalized to the case of doubly excited states \((N\ell, n\ell', 2\sigma^\pm, L^\pi, Z)\) as follows:
\[
Z^\ast = Z \left[ 1 - \beta(N\ell, n\ell', 2\sigma^\pm, L^\pi, Z) \right]^{\frac{1}{2}}
\]  
(32)
\[ E(1^2S) = -Z^2 \text{Ryd} - Z^2 \left[ 1 - \beta(1S, Z) \right]^2 \text{Ryd} \quad (33) \]

In equation (33), the second term of the right-hand side gives the first ionization energy. As the lowest-energy
\[ E(N\ell, n\ell', 2s^{1+}L^{\ell}) = -Z^2 \left( \frac{1}{N^2} + \frac{1}{n^2} \left[ 1 - \beta(N\ell, n\ell', 2s^{1+}L^{\ell}, Z) \right]^2 \right) \text{Ryd} \quad (34) \]

To calculate the energies, we used

For $2s^{1+}L^{\ell}$ states, $C_3 = 2.5$ and this

To calculate the energies, we used

For the $2s^{1+}L^{\ell}$ and $2p^{1+}L^{\ell}$ states, $C_3 = 8$ and $C_4$ it

Table 1. Energy doubly excited $2s^{1+}L^{\ell}$ states of He-like systems (Z=2-10). The energies E are in eV.

<table>
<thead>
<tr>
<th>Z</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.80</td>
<td>0.663459</td>
<td>16.306187</td>
<td>1.50</td>
<td>0.729604</td>
<td>14.978090</td>
<td>0.60</td>
<td>0.743241</td>
</tr>
<tr>
<td>3</td>
<td>2.20</td>
<td>0.682478</td>
<td>38.732255</td>
<td>1.85</td>
<td>0.736960</td>
<td>34.967790</td>
<td>0.70</td>
<td>0.681944</td>
</tr>
<tr>
<td>4</td>
<td>2.65</td>
<td>0.723437</td>
<td>70.652667</td>
<td>2.10</td>
<td>0.705284</td>
<td>63.653537</td>
<td>0.80</td>
<td>0.659242</td>
</tr>
<tr>
<td>5</td>
<td>3.00</td>
<td>0.723104</td>
<td>112.688184</td>
<td>2.50</td>
<td>0.746761</td>
<td>100.418583</td>
<td>0.90</td>
<td>0.651543</td>
</tr>
<tr>
<td>6</td>
<td>3.30</td>
<td>0.712025</td>
<td>164.723696</td>
<td>3.20</td>
<td>0.874885</td>
<td>144.787414</td>
<td>1.10</td>
<td>0.722112</td>
</tr>
<tr>
<td>7</td>
<td>3.60</td>
<td>0.705430</td>
<td>226.567535</td>
<td>3.60</td>
<td>0.886240</td>
<td>198.454455</td>
<td>1.20</td>
<td>0.715839</td>
</tr>
<tr>
<td>8</td>
<td>3.90</td>
<td>0.701023</td>
<td>298.229436</td>
<td>3.90</td>
<td>0.870421</td>
<td>260.915524</td>
<td>1.20</td>
<td>0.659631</td>
</tr>
<tr>
<td>9</td>
<td>4.25</td>
<td>0.707015</td>
<td>379.483459</td>
<td>4.25</td>
<td>0.868153</td>
<td>331.746820</td>
<td>1.20</td>
<td>0.617393</td>
</tr>
<tr>
<td>10</td>
<td>4.55</td>
<td>0.702858</td>
<td>470.812844</td>
<td>4.55</td>
<td>0.855679</td>
<td>411.248041</td>
<td>1.20</td>
<td>0.585029</td>
</tr>
</tbody>
</table>

Table 2. Energy doubly excited $2s^{1+}P^0$ states of He-like systems (Z=2-10). The energies E are in eV.

<table>
<thead>
<tr>
<th>Z</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
<th>$2s$</th>
<th>$2p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.51</td>
<td>0.759983</td>
<td>18.849532</td>
<td>1.23</td>
<td>0.957725</td>
<td>15.247958</td>
<td>0.87</td>
<td>0.943344</td>
</tr>
<tr>
<td>3</td>
<td>1.72</td>
<td>0.751725</td>
<td>47.810694</td>
<td>1.42</td>
<td>0.926908</td>
<td>37.109854</td>
<td>1.04</td>
<td>0.965049</td>
</tr>
<tr>
<td>4</td>
<td>1.92</td>
<td>0.755942</td>
<td>90.318773</td>
<td>1.60</td>
<td>0.920405</td>
<td>68.760013</td>
<td>1.18</td>
<td>0.964131</td>
</tr>
<tr>
<td>5</td>
<td>2.10</td>
<td>0.759537</td>
<td>146.474359</td>
<td>1.80</td>
<td>0.942207</td>
<td>109.927495</td>
<td>1.31</td>
<td>0.968035</td>
</tr>
<tr>
<td>6</td>
<td>2.25</td>
<td>0.757718</td>
<td>215.925692</td>
<td>2.00</td>
<td>0.967647</td>
<td>160.735552</td>
<td>1.42</td>
<td>0.967884</td>
</tr>
<tr>
<td>7</td>
<td>2.40</td>
<td>0.762678</td>
<td>299.123270</td>
<td>2.10</td>
<td>0.945499</td>
<td>222.085794</td>
<td>1.51</td>
<td>0.962342</td>
</tr>
<tr>
<td>8</td>
<td>2.50</td>
<td>0.755721</td>
<td>396.187122</td>
<td>2.25</td>
<td>0.956707</td>
<td>292.685734</td>
<td>1.60</td>
<td>0.965728</td>
</tr>
<tr>
<td>9</td>
<td>2.60</td>
<td>0.754630</td>
<td>506.673703</td>
<td>2.40</td>
<td>0.971378</td>
<td>372.960541</td>
<td>1.67</td>
<td>0.963922</td>
</tr>
<tr>
<td>10</td>
<td>2.70</td>
<td>0.757748</td>
<td>630.596387</td>
<td>2.50</td>
<td>0.970357</td>
<td>463.401665</td>
<td>1.73</td>
<td>0.963311</td>
</tr>
</tbody>
</table>
Based on the processing of the calculations, energy conversion of 1 a.u. = 2 Ry = 27.211385 eV was used. For the calculation of doubly excited states for Helium-like ions, several authors have used different methods. Thus, Ho [3, 23, 31] used the method of complex rotation convoluted with a wave function of Hylleraas type, Dieng [4] used Special Forms of Hylleraas-Type Wave Functions, Ivanov and Safronova [24] performed calculation using double sum method over the complete hydrogen spectrum, Sakho [25], Lipsky et al. [26], Ray and P. K. Mukherjee [27], Ho [3, 23, 31], Drake and Dalgaro [29], Seminario and Sanders [30], Sakho [16, 32], Lipsky et al. [26], Ray and P. K. Mukherjee [27], Kar and Ho [28] for the 2s2p 1S0, 2s3p 1P0, 2p3p 1S0, 2p3p 1P0, 2p3p 1D0 states. For these states, we note generally a quite good agreement.

In Table 7, results of 2s2p 1P0, 2s3p 1P0, 2p3p 1P0 states were compared with those of Ho [23, 31], Sakho [25, 32], Drake and Dalgaro [29], Dieng [4], Seminario and Sanders [30], Lipsky et al. [26]. For these states, we note generally a quite good agreement and little discrepancy with Dieng results.

We have also compared in Table 8, results with those from Ho and A. Bathia [3], Dieng [4], Sakho [25], Lipsky et al. [26], Ray and P. K. Mukherjee [27] for the 2p3p 1L1, 2p4p 1L1 states. We note good consistency.

In summary, we have calculated the singlet and triplet doubly excited states energies using a new wave function to four terms. We note here generally a satisfactory agreement between the present results and the other available calculations and we find a good agreement.
### Table 5. A comparison of the doubly excited $2s2p^{++}1^{2}S^0$, $2s4p^{++}1^{2}S^0$ states of He-like systems ($Z = 2–10$) with other results. The energies $E$ are in eV.

<table>
<thead>
<tr>
<th>$Z$</th>
<th>states</th>
<th>$E$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>16.36187</td>
</tr>
<tr>
<td>3</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>16.05267</td>
</tr>
<tr>
<td>4</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>15.16574</td>
</tr>
<tr>
<td>5</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>16.063152</td>
</tr>
<tr>
<td>6</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>16.643595</td>
</tr>
<tr>
<td>7</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>16.196223</td>
</tr>
<tr>
<td>8</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>14.978890</td>
</tr>
<tr>
<td>9</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>15.993410</td>
</tr>
<tr>
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<td>15.098242</td>
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<td>12</td>
<td>$2s2p^{++}1^{2}S^0$</td>
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<td>14.941770</td>
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<tr>
<td>14</td>
<td>$2s2p^{++}1^{2}S^0$</td>
<td>15.930095</td>
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<table>
<thead>
<tr>
<th>$Z$</th>
<th>states</th>
<th>$E$ (eV)</th>
</tr>
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<tbody>
<tr>
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<td>$2s4p^{++}1^{2}P^0$</td>
<td>18.872191</td>
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<td>$2s4p^{++}1^{2}P^0$</td>
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</tr>
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<td>$2s4p^{++}1^{2}P^0$</td>
<td>15.247958</td>
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<td>$2s4p^{++}1^{2}P^0$</td>
<td>15.347221</td>
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### Table 6. A comparison of the doubly excited $2s2p^{1}P^0$, $2s3p^{1}P^0$, $2s4p^{1}P^0$ states of He-like systems ($Z = 2–10$) with other results. All energies are given in eV.

<table>
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</tr>
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# Footnotes

Table 7. A comparison of the doubly excited $2s2p^3p^0$, $2s3p^3p^0$, $2s4p^3p^0$ states of He-like systems ($Z = 2–10$) with other results. All energies are given in eV.

<table>
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<th>$Z$</th>
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<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
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<th>10</th>
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<tbody>
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</tbody>
</table>

Table 8. A comparison of the doubly excited $2p3p^3p^0$, $2p4p^3p^0$ states of He-like systems ($Z = 2–10$) with other results. All energies are given in eV.

<table>
<thead>
<tr>
<th>states</th>
<th>$Z$</th>
<th>2</th>
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<th>4</th>
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<tbody>
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<td>223.263429</td>
<td>294.299849</td>
<td>375.162008</td>
<td>465.851021</td>
</tr>
</tbody>
</table>

References:
- Present work, + Ho [31], 1 Ho [23] for 2p3p state, * Ho [3] for 2s4p state, # Dieng [4], † Sakho [32] for 2s3p state and
- ‡ Sakho [25] for 2s4p state, § Lipsky [28], ¶ Ray [27], ‡ Kar [28], † Ivanov [24], # Drake [29], ‡ Seminario [30]
4. Conclusion

The method of Hylleraas was successfully applied by himself in the calculation of the energy of the ground state of helium and its isoelectronic series.

To expand this application to calculate the total energy of atomic systems in the doubly excited states we used a new wave function correlated with four terms adapted to the description of these conditions and using the method of Screen Constant by Unit Nuclear Charge, which has the advantage of leading to very accurate results as was the case in several approximation methods applied to the treatment of the properties of atomic systems with two electrons. [33-34]

It has been demonstrated the possibilities to use the screening constant by unit nuclear charge method in the study of $1s^2s^2 S$ , $1s^2p^2 P$ and $1s^2p^2 D$ doubly excited states in the helium-like ions in the framework of a variational procedure. Thus, a new correlated wave function is performed and results obtained are shown by the comparison with various available theoretical literature values (See Table 5-8). One can notice that, the merit of the Screening Constant by Unit Nuclear Charge method is to give the possibilities to calculate accurate energies for doubly excited states in two electron systems using a variational procedure.

References