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Variational Calculation of the Doubly-Excited States Nsnp of He-Like Ions via the Modified Atomic Orbitals Theory

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Abstract

In this paper, we have declined the formalism of the method of the Modified Atomic Orbital Theory (MAOT) applied to the calculations of energies of doubly excited states $2snp$, $3snp$, and $4snp$ Helium-like systems. Then we also applied the variational procedure of the Modified Atomic Orbital Theory to the computations of total energies, excitation energies of doubly-excited states $2snp$, $3snp$, $4snp$ types of Helium-like systems. The results obtained in this work are in good agreement with the experimental and theoretical values available.

Keywords

Modified Atomic Orbital Theory, Doubly Excited States, Excitation Energy, Helium-Like Systems

1. Introduction

Much theoretical research has revealed that the helium atom exhibits a strong electron-electron correlation. Since the early experiment by Madden and Codling [1], Madden and Ederer [2], and theoretical explanation by Cooper *et al.* [3], doubly-excited states of helium-like atoms have been the target of a number of theoretical approaches. The increasing interest of physicists in these studies over the years is connected with the understanding of collisional and radiational processes which take place in hot astrophysical and laboratory plasma [4]. The greatest attention has been concentrated on the study of doubly-excited states [5]. Some of these doubly-excited states in two-electron systems have been iden-

tified in the solar flare [6] and in the solar corona [7] and revealed experimentally by the studies of double Rydberg resonances in negative ions of rare gases [8] [9]. The investigations of the intrashell S states of two-electron systems are advanced and due to the group theoretical method [10] [11] which allowed intrashell states to be approximately classified and some of these properties were studied [12] [13].

So, most atomic spectra can be treated in term of singly excitation of singly or mixed configurations [14] [15]. After Herrick and Sinanoglu [11], higher-energy Rydberg envelopes contain doubly-excited states which are generally labelled in the usual spectroscopic notation $(Nl, nl')^{2S+1}L^{\pi}$ with $n = N, N+1, \cdots$. In these notations, N and n denote respectively the principal quantum numbers of the inner and the outer electron, l and l' are respectively orbital quantum numbers, S the total spin, L the total angular momentum and π the parity of the system.

Various methods have been performed to understand electron-electron correlation effects in doubly $(Nl, nl')^{2S+1}L^{\pi}$ excited states of He-like systems. Although many accurate data have been tabulated for these doubly excited states, the methods used require in general, complexity in the Variationnal procedure along with the use of computational codes.

Many theoretical studies have been done on doubly-excited states $(Nl, nl')^{2S+1}L^{\pi}$. Among these methods, we have the theoretical and experimental methods [16]-[23]. The variational method of time-independent perturbation from Ray and Mukherjee was applied for the calculation of the total energies of the $2s^2$, $2p^2$ and $3d^2$ states of He, Li^+, Be^{2+}, and B^{3+} [24]. Sakho used the semi-empirical procedure of the Screening Constant by Unit Nuclear Chargemethod (SCUNC) to calculate the energies of doubly excited states $(Nsnp)$ ^1P_o helium-like systems [25].

In all these ab initio methods, energies of $(Nl, nl')^{2S+1}L^{\pi}$ doubly-excited states of *He* isoelectronic sequence can't be expressed in an analytical formula. In addition, most of these preceding methods require large basis-set calculations involving a fair amount of mathematics complexity.

The Modified Atomic Orbital Theory is a purely theoretical method initiated by Sakho [26]. This theory stems from Slater's orbital theory [27]. This theory (MAOT) has been known for its simplicity, as it is a very suitable calculation method that has yielded enormous results from simple semi-empirical formulas without resorting to a computer program in solving resonant photoionization problems. It was subsequently that Sakho [25] studied the resonance energies of the Rydberg series of $2s^22p^4$ ($^1D_2$) ns, nd, $2s^22p^4$ ($^1S_0$) ns, nd, and $2s^22p^5$ ($^3P_2$) states from of the metastable $2s^22p^5$ ($^2P_{1/2}$) state and the ground $2s^22p^5$ ($^2P_{3/2}$) state of the Ne$^+$ ion. Thus the variational principle, which is a purely theoretical method, takes advantage of the principle of variation. This variational method is a computational technique to provide approximate solutions to solving the Schrödinger equation. In the following, after a brief review of Slater's orbital theory, we apply for the first time the variational procedure of the Modified

Atomic Orbitals Theory to the calculations of total energies, excitation energies of doubly excited 2s*n*p, 3s*n*p, 4s*n*p states of types helium-like systems. This procedure consists of determining the variational parameter α and the screening constant σ, from the construction of a correlated wave function.

2. Theory

2.1. Brief Description of the Modified Atomic Orbitals Theory

In the context of the Modified Atomic Orbitals Theory (MAOT), the total energy of a $(\nu\ell)$—given orbital is expressed as Rydberg units [28].

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

(1)

For the $(Nl, nl')^{2S+1}L^\pi$ doubly excited states, the total energy of an atomic system of many M electrons is expressed as follows

$$E = -\sum_{i=1}^{M} \frac{\left[Z - \sigma_i\left(^{2S+1}L^\pi\right)\right]^2}{\nu_i^2}.$$

(2)

2.2. Construction of the Wave Function

In the construction of the correlated wave function, a product of hydrogen-type wave functions is performed in which variational parameters are introduced. Thus, in the case of atomic systems, these criteria are generally determined by the screen effects exerted by the electrons on each other by the spin-orbit interaction, etc.

The hydrogen wave functions for $|n, l, m_l\rangle$ states are radial and have the same shape. They are non-normed and it's obtained from the radial coordinates (r) and an exponential factor.

So for different states, we get:

For 4s ($I = 0$):

$$R_{4,0}(r) = \frac{24}{96} \times \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \times \left(1 - \frac{3 \times Z}{4 \times a_0} \times r + \frac{Z^2}{8 \times a_0^2} \times r^2 - \frac{Z^3}{192 \times a_0^3} \times r^3\right) \times e^{-\frac{Z \times r}{4 \times a_0}}$$

(3)

For 4p ($I = 1$):

$$R_{4,1}(r) = \frac{5}{16\sqrt{2}} \times \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \times \left(\frac{Z}{a_0} \times r - \frac{1}{4} \times \frac{Z^2}{a_0^2} \times r^2 + \frac{1}{80} \times \frac{Z^3}{a_0^3} \times r^3\right) \times e^{-\frac{Z \times r}{4 \times a_0}}$$

(4)

For 3s ($I = 0$):

$$R_{3,0}(r) = \frac{1}{3\sqrt{3\pi}} \times \left(\frac{z}{a_0}\right)^{\frac{3}{2}} \times \left(1 - \frac{2}{3} \times \frac{Z}{a_0} \times r + \frac{2}{27} \times \frac{Z^2}{a_0^2} \times r^2\right) \times e^{-\left(\frac{Z \times r}{3 \times a_0}\right)}$$

(5)

For 3p ($I = 1$):

$$R_{3,1}(r) = \frac{2 \times \sqrt{2}}{27 \times \sqrt{\pi}} \times \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \times \left(\frac{Z}{a_0} \times r - \frac{Z^2}{6 \times a_0^2} \times r^2\right) \times e^{-\left(\frac{Z \times r}{3 \times a_0}\right)}$$

(6)

For 2s ($l = 0$):

$$R_{2,0}(r) = \frac{2}{4 \times \sqrt{2\pi}} \times \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \times \left(1 - \frac{Z}{2 \times a_0} \times r\right) \times e^{-\left(\frac{Z \times r}{2 \times a_0}\right)} \tag{7}$$

For 2p ($l = 1$):

$$R_{2,1}(r) = \frac{1}{4 \times \sqrt{2\pi}} \times \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \times \left(\frac{Z}{a_0} \times r\right) \times e^{-\left(\frac{Z \times r}{2 \times a_0}\right)} \tag{8}$$

To build the wave functions of $(Nl, nl')^{2S+1}L^{\pi}$ type, the product of the radial portions $R_{n,l}(r)$ is produced while considering the electrons (1) and (2) heliumoid systems, whose radial coordinates are respectively r_1 and r_2. As part of the independent particle model where electronic correlation phenomena are neglected, (Coulombian repulsion, spin-orbit interaction, etc.), the product of the functions is given as follows:

For the function 2s2p:

$$2s = \left(1 - \frac{Z}{2 \times a_0} \times r_1\right) \times e^{-\left(\frac{Z \times r_1}{2 \times a_0}\right)} \quad \text{and} \quad 2p = \left(\frac{Z}{a_0} \times r_2\right) \times e^{-\left(\frac{Z \times r_2}{2 \times a_0}\right)}$$

$$\Psi(2s2p) = \left[\left(1 - \frac{Z}{2 \times a_0} \times r_1\right) \times \left(\frac{Z}{a_0} \times r_2\right)\right] \times e^{-\frac{Z}{2 \times a_0} \times r_1} \times e^{-\frac{Z}{2 \times a_0} \times r_2} \tag{9}$$

For the function 3s3p:

$$3s = \left(1 - \frac{2 \times Z}{3 \times a_0} \times r_1 + \frac{2 \times Z^2}{27 \times a_0^2} r_1^2\right) \times e^{-\left(\frac{Z}{3 \times a_0} \times r_1\right)} \quad \text{and}$$

$$3p = \left(\frac{Z}{a_0} \times r_2 - \frac{Z^2}{6 \times a_0^2} \times r_2^2\right) \times e^{-\left(\frac{Z}{3 \times a_0} \times r_2\right)}$$

$$\Psi(3s3p) = \left(\left(1 - \frac{2 \times Z}{3 \times a_0} \times r_1 + \frac{2 \times Z^2}{27 \times a_0^2} r_1^2\right) \times \left(\frac{Z}{a_0} \times r_2 - \frac{Z^2}{6 \times a_0^2} \times r_2^2\right)\right)$$
$$\times e^{-\left(\frac{Z}{3 \times a_0} \times r_1\right)} \times e^{-\left(\frac{Z}{3 \times a_0} \times r_2\right)} \tag{10}$$

For the function 4s4p:

$$4s = \left(1 - \frac{3 \times Z}{4 \times a_0} \times r + \frac{Z^2}{8 \times a_0^2} \times r^2 - \frac{Z^3}{192 \times a_0^3} \times r^3\right) \times e^{-\left(\frac{Z \times r_1}{4 \times a_0}\right)}$$

$$4p = \left(\frac{Z}{a_0} \times r - \frac{1}{4} \times \frac{Z^2}{a_0^2} \times r^2 + \frac{1}{80} \times \frac{Z^3}{a_0^3} \times r^3\right) \times e^{-\left(\frac{Z \times r_2}{4 \times a_0}\right)}$$

$$\Psi(4s4p) = \left(\left(1 - \frac{3 \times Z}{4 \times a_0} \times r_1 + \frac{Z^2}{8 \times a_0^2} \times r_1^2 - \frac{Z^3}{192 \times a_0^3} \times r_1^3\right)\right.$$
$$\left. \times \left(\frac{Z}{a_0} \times r_2 - \frac{1}{4} \times \frac{Z^2}{a_0^2} \times r_2^2 + \frac{1}{80} \times \frac{Z^3}{a_0^3} \times r_2^3\right)\right) \times e^{-\left(\frac{Z \times r_1}{4 \times a_0}\right)} \times e^{-\left(\frac{Z \times r_2}{4 \times a_0}\right)} \tag{11}$$

Taking into account the phenomena of electron-electron correlation effects occurring in *He*-like systems, the nuclear charge of the exponential factor is substituted in favor of the effective charge Z^*, and in atomic unit, the Bohr radius $a_0 = 1$.

So these functions become:

For the wave function 2s*n*p:

$$\Psi(2\text{snp}) = \left(\left(1 - \frac{Z}{2 \times a_0} \times r_1\right) \times \left(\frac{Z}{a_0} \times r_2\right)\right) \times e^{-\frac{Z^*}{n}(r_1 + r_2)} \tag{12}$$

For the wave function 3s*n*p:

$$\Psi(3\text{snp}) = \left(\left(1 - \frac{2 \times Z}{3 \times a_0} \times r_1 + \frac{2 \times Z^2}{27 \times a_o^2} r_1^2\right) \times \left(\frac{Z}{a_0} \times r_2 - \frac{Z^2}{6 \times a_0^2} \times r_2^2\right)\right) \times e^{-\frac{Z^*}{n}(r_1 + r_2)} \tag{13}$$

For the wave function 4s*n*p:

$$\Psi(4\text{snp}) = \left(\left(1 - \frac{3 \times Z}{4 \times a_0} \times r_1 + \frac{Z^2}{8 \times a_0^2} \times r_1^2 - \frac{Z^3}{192 \times a_0^3} \times r_1^3\right)\right.$$
$$\left. \times \left(\frac{Z}{a_0} \times r_2 - \frac{1}{4} \times \frac{Z^2}{a_0^2} \times r_2^2 + \frac{1}{80} \times \frac{Z^3}{a_0^3} \times r_2^3\right)\right) \times e^{-\frac{Z^*}{n}(r_1 + r_2)} \tag{14}$$

where the effective charge number Z^* is given by:

$$Z^* = Z\left(1 - \frac{\sigma(Nl, nl')}{Z}\right) \tag{15}$$

With $\sigma(Nl, nl')$ the screen constant relating to these states.

2.3. Determining the Screen Constant

To determine the screen constant, we start from the relation:

$$E(\alpha) = \langle H \rangle(\alpha) = \frac{\langle \Psi(\alpha) | H | \Psi(\alpha) \rangle}{\langle \Psi(\alpha) | \Psi(\alpha) \rangle} \tag{16}$$

And Hamiltonian of the helium isoelectronic series in given by (in atomic units):

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \tag{17}$$

The average value of this expression (17), while using the closure relation reflecting the fact that the $|r_1, r_2\rangle$ kets are continuous bases in the state space of the two electrons:

$$\iint dr_1^3 dr_2^3 |r_1, r_2\rangle\langle r_1, r_2| = \mathbb{1} \tag{18}$$

From this relation we can from (21):

$$E(\alpha)\iint d^3r_1 d^3r_2 \langle \Psi(\alpha) \| r_1, r_2 \rangle \times \langle r_1, r_2 \| \Psi(\alpha) \rangle$$
$$= \iint d^3r_1 d^3r_2 \langle \Psi(\alpha) \| r_1, r_2 \rangle \hat{H} \langle r_1, r_2 \| \Psi(\alpha) \rangle \tag{19}$$

The development of (19) gives:

$$E(\alpha) \iint d^3 r_1 d^3 r_2 \Psi(r_1, r_2, \alpha) \times \Psi^*(r_1, r_2, \alpha)$$
$$= \iint d^3 r_1 d^3 r_2 \Psi(r_1, r_2, \alpha) \hat{H} \Psi^*(r_1, r_2, \alpha) \tag{20}$$

The normalization constant denoted *N* is given by:

$$NE(\alpha) = \iint d^3 r_1 d^3 r_2 \Psi(r_1, r_2, \alpha) \hat{H} \Psi^*(r_1, r_2, \alpha) \tag{21}$$

And from this relation (24), we obtain:

$$N = \iint d^3 r_1 d^3 r_2 \left| (r_1, r_2, \alpha) \right|^2 \tag{22}$$

To facilitate the development of these expressions, we made a change of variable of some parameters of the Equation (20). It was later that we posed in elliptical coordinates:

$$s = (r_1 + r_2); t = (r_1 - r_2); u = r_{12} \tag{23}$$

And the element of elementary volume gives:

$$d\tau = dr_1^3 dr_2^3 = 2\pi^2 (s^2 - t^2) u \, ds \, dt \, du \tag{24}$$

Applying these changes of variables in Equation (23) the preceding expression of the normalization constant denoted *N* is in elliptic coordinate:

$$NE(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 + \left(\frac{\partial \Psi}{\partial t} \right)^2 + \left(\frac{\partial \Psi}{\partial u} \right)^2 \right] + 2 \left(\frac{\partial \Psi}{\partial u} \right) \right.$$
$$\left. \times \left[s(u^2 - t^2) \frac{\partial \Psi}{\partial s} + t(s^2 - u^2) \frac{\partial \Psi}{\partial t} \right] - \Psi^2 \left[4Zsu - s^2 + t^2 \right] \right\} \tag{25}$$

Since we did not take into account the Coulomb repulsion, so: $\dfrac{\partial \Psi}{\partial u} = 0$.

The normalization constant becomes:

$$NE(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 + \left(\frac{\partial \Psi}{\partial t} \right)^2 \right] - \Psi^2 \left[4Zsu - s^2 + t^2 \right] \right\} \tag{26}$$

To determine the values of the screen constant σ and the variational parameter α, we start from this equation, which is the sum of three integral data as follows:

$$NE(\alpha) = E_1(\alpha) + E_2(\alpha) + E_3(\alpha) \tag{27}$$

The development of this expression (27) makes it possible to obtain the value of σ and α by the formula:

$$\frac{dE(\alpha_i)}{d\alpha_i} = 0 \tag{28}$$

The expressions corresponding to $E_1(\alpha)$, $E_2(\alpha)$, and $E_3(\alpha)$, are:

$$E_1(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt \, u(s^2 - t^2) \times \left(\frac{\partial \Psi}{\partial s} \right)^2 \tag{29}$$

$$E_2(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt\, u(s^2 - t^2) \times \left(\frac{\partial \Psi}{\partial t}\right)^2 \tag{30}$$

$$E_3(\alpha) = -\int_0^\infty ds \int_0^s du \int_0^u dt\,\left[4Zsu - s^2 + t^2\right]\Psi^2 \tag{31}$$

The normalization constant is as follows:

$$N = \int_0^\infty ds \int_0^s du \int_0^u dt\, u(s^2 - t^2) \times \Psi^2 \tag{32}$$

With these changes of variables, the correlated wave functions of the states 2s*n*p, 3s*n*p, and 4s*n*p become:

$$\Psi(2s2p) = -\frac{1}{8} \times \left((s-t) \times (s \times z + t \times z - 4)\right) \times e^{-\alpha s} \tag{33}$$

$$\Psi(3s3p) = \frac{1}{1296} \times \Big[z \times (s-t) \times (s \times z - t \times z - 12) \times \big(s^2 \times z^2 + 2 \times s \times t \times z^2 \\ -18 \times s \times z + t^2 \times z^2 - 18 \times t \times z + 54\big)\Big] \times e^{-\alpha s} \tag{34}$$

$$\Psi(4s4p) = -\frac{1}{983040} \times \Big(z \times (s-t) \times \big(s^2 \times z^2 - 2 \times s \times t \times z^2 - 40 \times s \times z \\ + t^2 \times z^2 + 40 \times t \times z + 320\big) \times \big(s^3 \times z^3 + 3 \times s^2 \times t \times z^3 - 48 \times s^2 \times z^2 \\ + 3 \times s \times t^2 \times z^3 - 96 \times s \times t \times z^2 + 576 \times s \times z + t^3 \times z^3 \\ - 48 \times t^2 \times z^2 + 576 \times t \times z - 1536\big)\Big) \times e^{-\alpha s} \tag{35}$$

3. Results and Discussions

In this part, the procedure consists of determining the final expressions of energies, the value of the variational parameter α, and the screen constant σ. Since the calculations used are very complex, and require a lot of changes of variables, with matrices to be manipulated, we have found it necessary to make a first call to a computer program with the software matlab. In this program, we first defined the parameter *s*, *t*, *u*, *α*, and *z* of Equation (23), the expression of the derivative as a function of each parameter, and the square of its derivatives. In a second step, the expressions of (E_1, E_2, E_3 and N) of the Equations (29)-(32), as well as their factorials were defined and detailed expression by expression. Then, to simplify some parameters, a matrix calculation was carried out in this program, and relations between these matrices were made to obtain a simple expression of the Equation (27) in order to apply the formula of the Equation (28) to have the approximate values of the screen constant σ and the variational parameter α.

3.1. Expression of the Total Energies

In the case of the variational calculation of the Modified Atomic Orbital theory (MAOT, the expression of the total energy of the doubly-excited states (*Ns*np) of an orbital is given by the formula (in Rydberg):

$$E(N\text{s}n\text{p}) = -\left(\frac{(Z-\sigma(n\text{s}))^2}{N^2}\right) - \left(\frac{(Z-\sigma(n\text{p}))^2}{n^2}\right) \tag{36}$$

With $N \neq n$ and $\sigma(n\text{s}) = \sigma(n\text{p})$.

In some cases, a corrective factor may be added to this expression to obtain results that are closer to those found in the literature consulted.

Thus the expressions of the states 2s*n*p, 3s*n*p, and 4s*n*p are detailed as follows:

- For the state 2s*n*p:

$$E(2\text{s}2\text{p}) = -\left(\frac{(Z-\sigma(n\text{s}))^2}{N^2}\right) - \left(\frac{(Z-\sigma(n\text{p}))^2}{n^2}\right) \tag{37}$$

With $\sigma(n\text{s}) = \sigma(n\text{p})$ and $N = n$.

- For the state 3s*n*p:

$$E(3\text{s}3\text{p}) = -\left(\frac{(Z-\sigma(n\text{s}))^2}{N^2}\right) - \left(\frac{(Z-\sigma(n\text{p}))^2}{n^2}\right) \tag{38}$$

With $\sigma(n\text{s}) = \sigma(n\text{p})$ et $N = n$.

- For the state 4s*n*p:

$$E(4\text{s}4\text{p}) = -\left(\frac{(Z-\sigma(n\text{s}))^2}{N^2}\right) - \left(\frac{(Z-\sigma(n\text{p}))^2}{n^2}\right) \tag{39}$$

With $\sigma(n\text{s}) = \sigma(n\text{p})$ and $N = n$.

3.2. Expression of the Variational Parameter α

The determination of the variational parameter α comes from the expression (28) with:

$$E(\alpha_i) = \sum_{i=1}^{3}\left(\frac{E_i}{N}\right) \tag{40}$$

Thus the calculation program is presented in the **Appendix**, and the variational parameter α of the states 2s2p, 3s3p and 4s4p is given as follows:

$$\alpha = \frac{n+l+l'}{n}Z\left(1 - \frac{\sigma(Nl, nl')}{Z}\right) \tag{41}$$

For the state 2s2p:

$$\alpha_2(2\text{s}2\text{p}) \approx \frac{3}{2}Z\left(1 - \frac{1}{2}\times\frac{1}{Z}\right) \tag{42}$$

With $\sigma(2\text{s}2\text{p}) = 0.5$.

For the state 3s3p:

$$\alpha_3(3\text{s}3\text{p}) \approx \frac{4}{3}Z\left(1 - \frac{3}{12}\times\frac{1}{Z}\right) \tag{43}$$

With $\sigma(3\text{s}3\text{p}) = 0.25$.

For the state 4s4p:

$$\alpha_4\left(4\text{s}4\text{p}\right) \approx \frac{5}{4}Z\left(1-\frac{3}{7}\times\frac{1}{Z}\right) \tag{44}$$

With $\sigma\left(4\text{s}4\text{p}\right) = 0.428$.

3.3. Results and Discussion

In this work, the results obtained are compared with those found in the theoretical and experimental literature. We have calculated the total energies of the states (3snp ^{1}Pº), (2snp ^{1}Pº), (4snp ^{1}Pº) as well as the excitation energies of the states (3snp ^{1}Pº), (2snp ^{1}Pº), (4snp ^{1}Pº). For the states (3snp ^{1}Pº) the total energies are given in Rydberg and in eV, shown in Table 1 (1 eV = 13.605698 Ryd) shown in Table 2. For the (2snp ^{1}Pº), (4snp ^{1}Pº) states, their results are given in eV and represented in Table 3 and Table 4 respectively. Equations (37), (38), (39) have been used for the calculation of its total states energies (3snp ^{1}Pº), (2snp ^{1}Pº), (4snp ^{1}Pº) respectively. About excitations energies, we have taken the energies of the ground state given by Frankowski and Pekeris [29]. These energies are given in ua (1 ua = 2 Rydberg) their values are given as follows: He (−2.90372), Li$^+$ (−7.27991), Be^{2+} (−13.65556), Be^{3+} (−22.03097).

In Tables 1-4, we used the variational computation of the modified atomic orbitals theory (MAOT) of the energies doubly-excited states (3snp ^{1}Pº), (2snp ^{1}Pº), (4snp ^{1}Pº). We compared the results obtained with theoretical results for all of these states, and experimental results existing only for the (3s3p ^{1}Pº), (2s2p ^{1}Pº), helium (He) states of Kossmann *et al.* [17], (2s2p ^{1}Pº), lithium (Li$^+$) from Diehl *et al.* [19], and (4s4p ^{1}Pº) from Woodru *et al.* [30]. The theoretical results to which we have compared our results are those of Sakho *et al.* [25], Ivanov and Safronova [15], Drake and Dalgarno [22], Ho [18], Biaye *et al.* [21], Bachau

Table 1. The total energies of the doubly excited states of (Nsnp) ^{1}Pº helium-like systems (Z = 2 to 10) in Rydberg (1 Ryd = 13.60569 eV).

States		Z								
		2	3	4	5	6	7	8	9	10
3s3p ^{1}Pº	−E^p	0.68056	1.68056	3.12500	5.01389	7.34722	10.12500	13.34722	17.01389	21.12500
	−E^s	0.66054	1.64784	3.07958	4.95577	7.27640	10.04147	13.25099	16.90496	21.00337
	−E^a	0.67140	1.659 40	3.09000	4.96600	7.28600	10.04800	13.25600	16.91000	21.00000
	−E^b	0.66268	1.67395	3.15417	5.10468	7.52607	10.41871	13.78253	17.61787	21.92494
3s4p ^{1}Pº	−E^p	0.53168	1.31293	2.44141	3.91710	5.74002	7.91016	10.42752	13.29210	16.50391
	−E^s	0.53206	1.31269	2.44053	3.91561	5.73790	7.90742	10.42415	13.28811	16.49930
	−E^a	0.54240	1.31960	2.44400	3.91400	5.73000	7.89600	10.40800	13.26600	16.47200
3s5p ^{1}Pº	−E^p	0.46278	1.14278	2.12500	3.40944	4.99611	6.88500	9.07611	11.56944	14.36500
	−E^s	0.47259	1.15756	2.14475	3.43416	5.02579	6.91965	9.11573	11.61403	14.41455

P: Present results obtained from Equation (38); s: (Sakho *et al.*, 2010) [26], a: (Bachau *et al.*, 1991) [20]; b: (Biaye *et al.*, 2005) [21].

Table 2. The total energies of the doubly excited states of (*Nsn*p) ¹Pᵒ types of helium-like systems (*Z* = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

States		Z								
		2	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
3s3p ¹Pᵒ	−Eᵖ	9.26	22.87	42.52	68.22	99.96	137.76	181.60	231.49	287.42
	−Eˢ	9.10	22.47	41.88	67.34	98.85	136.40	180.01	229.66	285.35
	−Eʰ	8.28	21.14	40.05	65.01	96.01	133.06	176.16	225.30	280.49
	−Eᵏ	9.10	22.33	42.04	67.52	99.03				
	−Eˡ	9.11	22.54	42.00	67.51					
	−Eⁱ	9.10								
3s4p ¹Pᵒ	−Eᵖ	7.23	17.86	33.22	53.29	78.10	107.62	141.87	180.85	224.55
	−Eˢ	7.66	18.42	33.90	54.10	79.03	108.68	143.06	182.16	225.98
3s5p ¹Pᵒ	−Eᵖ	6.30	15.55	28.91	46.39	67.98	93.68	123.49	157.41	195.45
	−Eˢ	7.02	16.58	30.25	48.03	69.93	95.94	126.05	160.05	198.63

P: Present results obtained from Equation (38); s: (Sakho *et al.*, 2008) [25]; h: (Ivanov and Safronova, 1993) [16]; i: experimental results (Kossmann *et al.*, 1988) [17]; k: (Wagué, 1987) [31]; l: (Lipsky *et al.*, 1977) [32].

Table 3. The total energies of the doubly excited states of (*Nsn*p) ¹Pᵒ types of helium-like systems (*Z* = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

States		Z								
		2	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
2s2p ¹Pᵒ	−Eᵖ	17.96	46.88	89.39	145.52	215.25	298.58	395.52	506.07	630.22
	−Eˢ	18.88	47.76	90.24	146.34	216.03	299.33	396.24	506.76	630.88
	Eᵃ	18.86	47.82	90.33	146.40	216.07	299.32	396.18	506.64	630.70
	−Eʰ	19.42	48.23	90.63	146.66	216.28	299.51	396.34	506.78	630.84
	−Eʲ	18.87	47.84	90.34	146.42	216.09	299.34	396.20	506.20	630.84
	−Eᶠ'ⁱ	18.88ⁱ	47.78*f*							
2s3p ¹Pᵒ	−Eᵖ	15.05	37.16	69.09	110.85	162.44	223.86	295.10	376.16	467.06
	−Eˢ	15.95	38.23	70.34	112.28	164.04	225.63	297.05	378.29	469.36
	−Eʰ	15.95	37.99	69.86	111.55	163.07	224.41	295.59	376.58	467.41

P: Present results obtained from Equation (37); s: (Sakho *et al.*, 2008) [25]; a: (Ho, 1980) [18]; h: (Ivanov and Safronova, 1993) [16]; i: experimental results (Kossmann *et al.*, 1988) [17]; f: Experimental data, (Diehl *et al.*, 1999) [19]; j: (Drake and Dalgarno, 1971) [22].

et al. [20], Sakho *et al.* [26], Wagué [31], Lipsky *et al.* [32].

Thus in **Table 1**, **Table 2**, containing the states (3snp ¹Pᵒ), we have calculated the total energies of doubly-excited states types (3s*n*p ¹Pᵒ) ranging from (*Z* = 2 to 10) using Equation (38).

The results found are in perfect agreement with those found in the theoretical and experimental literature consulted and quoted above. For the (3s3p ¹Pᵒ) helium (He) states, we compared our results with those obtained experimentally by

Kossman *et al.* [17], and the results obtained are in perfect agreement.

In **Table 3** and **Table 4**, containing the states (2snp ^{1}P^o), and (4s4p ^{1}P^o), we used the Equations ((37), (39)) respectively. Then we added to each of these equations a corrective factor to obtain results equivalent to those found in the theoretical and experimental. In **Table 3**, states (2snp ^{1}P^o), we calculated the total energies of doubly excited states of helium-like systems (Z = 2 to 10). Our results found are in good agreement with the theoretical results [16] [22] [25] and experimental [17] [19].

In **Table 4**, states (4s4p ^{1}P^o), we also calculated the total energies of doubly-excited states of helium-like systems (Z = 2 to 10). The results found are in

Table 4. The total energies of the doubly excited states of (Nsnp) ^{1}P^o types of helium-like systems (Z = 2 to 10). Results given in eV (1 Ryd = 13.60569 eV).

State		Z								
		2	3	4	5	6	7	8	9	10
4s4p ^{1}P^o	$-E^p$	5.24	12.91	23.98	38.46	56.33	77.61	102.29	130.37	161.85
	$-E^s$	5.35	13.03	24.10	38.58	56.46	77.75	102.43	132.03	162.00
	E^α	5.29	12.95	24.01	38.46	56.31	77.56	102.43	130.27	161.72
	$-E^m$	5.35								

P: Present results obtained from Equation (39); m: Experimental data, Woodruff and Samson (1982) [30].

Table 5. Excitation energies of the doubly excited states of (Nsnp) ^{1}P^o types of helium-like systems (Z = 2 to 5). Results given in eV (1 Ryd = 13.60569 eV; 1 ua = 2 Rydberg).

States		Z			
		2	3	4	5
2s2p ^{1}P^o	E^p	61.05	151.22	282.19	453.98
	E^s	60.13	150.34	281.35	453.15
	E^j	60.13			
	$E^{f,i}$	60.13^i	150.31^f		
2s3p ^{1}P^o	E^p	63.97	160.94	302.50	488.64
	E^s	63.06	159.87	301.25	487.21
3s3p ^{1}P^o	E^p	69.75	175.23	329.07	531.28
	E^s	69.91	175.63	330.54	532.15
	E^i	69.91			
3s4p ^{1}P^o	E^p	71.78	180.23	338.37	546.20
	E^s	71.35	179.68	337.69	545.39
3s5p ^{1}P^o	E^p	72.72	182.55	342.67	553.11
	E^s	71.99	181.52	341.34	551.46
4s4p ^{1}P^o	E^p	73.78	185.19	347.60	561.04
	E^s	73.66	185.07	347.49	560.91
	E^m	73.66			

perfect agreement with those found in the literature consulted.

In Table 5, we presented the excitation energies of the doubly-excited states of (Nsnp ^{1}P°) (N, $n \leq 5$) types of helium and its assimilated ions. They are calculated from the energies of the ground state given by Frankowski and Pekeris [29]. The results found in this table are in perfect agreement with the results found by the other authors.

4. Conclusion

In a global way, we applied the variational procedure of the modified atomic orbitals theory for the computation of total energies and excitation senergies doubly-excited states of the atomic system with several electrons. In order to achieve our results, we used a matlab program for the first time to reduce the complexity of the calculations. This program allowed us to determine the approximate expressions of the variational parameter, and of the screen constant.

Conflicts of Interest

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

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Appendix

Appendix A: Calculation Procedure for the Determination of the Radial Wave Function

The procedure for determining the radial wave function is given as follows:

$$R_{n,l}(r) = \left\{ \left(\frac{2Z}{na_0} \right)^3 \frac{(n-l-1)!}{2n\left[(n+l)! \right]^3} \right\}^{1/2} e^{-\frac{zr}{na_0}} \left(\frac{2Zr}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right) \qquad (A1)$$

The associated Laguerre polynomials are linked to the Laguerre polynomials $L_{n+l}(r)$ by the Rodrigue formula:

$$L_n^k(r) = (-1)\frac{d^k}{dr^k} L_n(r) \qquad (A2)$$

$$L_n(r) = e^r \frac{d^n}{dr^n} \left(r^n e^{-r} \right) \qquad (A3)$$

For different values of n and l, the Laguerre polynomials are mutually orthogonal, which then determines the orthogonality of the radial wave functions.

Let's give the example of the 4s wave function:

For the state 4s we have: $n = 4$, $l = 0$

$$L_{n+l}^{2l+1}\left(\frac{2Zr}{na_o} \right) = L_4^1\left(\frac{2Zr}{na_o} \right) \Rightarrow \frac{d}{dr}(L_4(r))\left(\frac{2Zr}{na_o} \right) \qquad (A4)$$

And;

$$L_4 = e^r \frac{d^4}{dr^4} \left(r^n e^{-r} \right) \qquad (A5)$$

By developing this expression, we get:

$$L_4(r) = e^r \frac{d^3}{dr^3} \left(4r^3 e^{-r} - r^4 e^{-r} \right) = e^r \frac{d^2}{dr^2} \left(12r^2 e^{-r} - 4r^3 e^{-r} - 4r^3 e^{-r} + r^4 e^{-r} \right)$$

$$L_4(r) = e^r \frac{d}{dr} \left(24re^{-r} - 12r^2 e^{-r} - 12r^2 e^{-r} + 4r^3 e^{-r} \right.$$
$$\left. -12r^2 e^{-r} + 4r^3 e^{-r} + 4r^3 e^{-r} - r^4 e^{-r} \right)$$

$$L_4(r) = e^r \left(24e^{-r} - 24re^{-r} - 24re^{-r} + 12r^2 e^{-r} - 24re^{-r} + 12r^2 e^{-r} \right.$$
$$+12r^2 e^{-r} - 4r^3 e^{-r} - 24re^{-r} + 12r^2 e^{-r} + 12r^2 e^{-r} - 4r^3 e^{-r}$$
$$\left. +12r^2 e^{-r} - 4r^3 e^{-r} - 4r^3 e^{-r} + r^4 e^{-r} \right)$$

$$L_4(r) = \left(24 - 96r + 72r^2 - 16r^3 + r^4 \right) \qquad (A6)$$

Then he comes:

$$L_4^1 = \frac{d}{dr} L_4(r) = 4\left(-24 + 36 \times r - 12 \times r^2 + r^3 \right) \qquad (A7)$$

Which give,

$$L_{n+l}^{2l+1}\left(\frac{2Z \times r}{na_0}\right) = L_4^1\left(\frac{2Z \times r}{na_0}\right)$$

$$= (-4) \times \left(-24 \times \left(\frac{2Z}{4a_0}\right)^0 + 36 \times r\left(\frac{2Z}{4a_0}\right)^1 - 12 \times r^2\left(\frac{2Z}{4a_0}\right)^2 + r^3\left(\frac{2Z}{4a_0}\right)^3\right) \tag{A8}$$

So the determination of the first part of the expression (A1)

$$\left\{\left(\frac{2Z}{na_0}\right)^3 \times \frac{(n-l-1)!}{2n \times \left[(n+1)!\right]^3}\right\}^{\frac{1}{2}}$$

For $n = 4$ and $l = 0$, we have:

$$\left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n \times \left((n+l)!\right)^3}\right\}^{\frac{1}{2}} = \left\{\left(\frac{Z}{2 \times a_0}\right)^3 \times \left(\frac{6}{8 \times 24^3}\right)\right\}^{\frac{1}{2}}$$

$$= \left\{\left(\frac{Z}{2 \times a_0}\right)^3 \times \left(\frac{3}{4 \times 24^3}\right)^{\frac{1}{2}}\right\} = \left\{\left(\frac{Z}{2 \times a_0}\right)^{\frac{3}{2}}\left(\frac{1}{96 \times \sqrt{2}}\right)\right\} = \left\{\frac{1}{4 \times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\} \tag{A9}$$

$$\left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n \times \left((n+l)!\right)^3}\right\}^{\frac{1}{2}} = \left\{\frac{1}{4 \times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\} \tag{A10}$$

Thus, starting from (A8) and (A10);

$$\left\{\frac{1}{4 \times 96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right\} \times (-4) \times \left(-24 + \frac{18 \times Zr}{a_0} - \frac{3 \times Z^2 r^2}{a_0^2} + \frac{Z^3 r^3}{8a_0^3}\right)$$

$$= \left[\frac{1}{96}\left(24 - \frac{18Z}{a_0}r + \frac{32Z^2}{a_0^2}r^2 - \frac{Z^3}{8a_0^3}r^3\right)\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\right] \tag{A11}$$

Simplifying by 24 we finally obtain the expression of the radial wave function 4s as follows:

$$R_{4,0} = \frac{24}{96}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(1 - \frac{3Z}{4a_0}r + \frac{Z^2}{8a_0^2}r^2 - \frac{Z^3}{192a_0^3}r^3\right)e^{-\frac{Z \times r}{4a_0}} \tag{A12}$$

By analogy the wave function 4p is given as follows:

$$R_{4,1} = \frac{5}{16\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(\frac{Z}{a_0}r - \frac{1}{4}\frac{Z^2}{a_0^2}r^2 + \frac{1}{80}\frac{Z^3}{a_0^3}r^3\right)e^{-\frac{Z \times r}{4a_0}} \tag{A13}$$

Appendix B: Principle of Determining the Screen Constant

To determine the screen constant, we start from the relation:

$$E(\alpha) = \langle H \rangle(\alpha) = \frac{\langle \Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle \Psi(\alpha)|\Psi(\alpha)\rangle} \tag{B1}$$

And the Hamiltonian H (in atomic unit) is:

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{z}{r_1} - \frac{z}{r_2} + \frac{1}{r_{12}} \tag{B2}$$

The average value of this expression (B2), while using the closure relation reflecting the fact that the $|r_1, r_2\rangle$ kets are continuous bases in the state space of the two electrons:

$$\iint dr_1^3 dr_2^3 |r_1, r_2\rangle \langle r_1, r_2| = \mathbb{1} \tag{B3}$$

From this relation we can from (B3):

$$E(\alpha)\iint d^3r_1 d^3r_2 \langle \Psi(\alpha)\|r_1, r_2\rangle \times \langle r_1, r_2\|\Psi(\alpha)\rangle$$
$$= \iint d^3r_1 d^3r_2 \langle \Psi(\alpha)\|r_1, r_2\rangle \hat{H}\langle r_1, r_2\|\Psi(\alpha)\rangle \tag{B4}$$

The development of (B4) gives:

$$E(\alpha)\iint d^3r_1 d^3r_2 \Psi(r_1, r_2, \alpha) \times \Psi^*(r_1, r_2, \alpha)$$
$$= \iint d^3r_1 d^3r_2 \Psi(r_1, r_2, \alpha)\hat{H}\Psi^*(r_1, r_2, \alpha) \tag{B5}$$

The normalization constant denoted N is given by:

$$NE(\alpha) = \iint d^3r_1 d^3r_2 \Psi(r_1, r_2, \alpha)\hat{H}\Psi^*(r_1, r_2, \alpha) \tag{B6}$$

And from this relation (B6), we obtain:

$$N = \iint d^3r_1 d^3r_2 |(r_1, r_2, \alpha)|^2 \tag{B7}$$

To facilitate the development of these expressions, we made a change of variable of some parameters of the Equation (B5). It was later that we posed in elliptical coordinates:

$$s = (r_1 + r_2); t = (r_1 - r_2); u = r_{12} \tag{B8}$$

And the element of elementary volume gives:
We know that, $\mathrm{d}\tau = dr_1^3 dr_2^3$

$$\mathrm{d}\tau = dr_1^3 dr_2^3 = 2\pi^2 (s^2 - t^2) u \mathrm{d}s \mathrm{d}t \mathrm{d}u \tag{B9}$$

Applying these changes of variables in Equation (B7) the preceding expression of the normalization constant denoted N is in elliptic coordinate:

$$NE(\alpha) = \int_0^\infty \mathrm{d}s \int_0^s \mathrm{d}u \int_0^u \mathrm{d}t \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial\Psi}{\partial s}\right)^2 + \left(\frac{\partial\Psi}{\partial t}\right)^2 + \left(\frac{\partial\Psi}{\partial u}\right)^2 \right] + 2\left(\frac{\partial\Psi}{\partial u}\right) \right.$$
$$\left. \times \left[s(s^2 - t^2)\frac{\partial\Psi}{\partial s} + t(s^2 - u^2)\frac{\partial\Psi}{\partial t} \right] - \Psi^2 \left[4Zsu - s^2 + t^2 \right] \right\} \tag{B10}$$

Since we did not take into account the Coulomb repulsion, so: $\dfrac{\partial\Psi}{\partial u} = 0$

The normalization constant becomes:

$$NE(\alpha) = \int_0^\infty \mathrm{d}s \int_0^s \mathrm{d}u \int_0^u \mathrm{d}t \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial\Psi}{\partial s}\right)^2 + \left(\frac{\partial\Psi}{\partial t}\right)^2 \right] - \Psi^2 \left[4Zsu - s^2 + t^2 \right] \right\} \tag{B11}$$

To determine the values of the screen constant σ and the variational parameter α, we start from this equation, which is the sum of three integral data as follows:

$$NE(\alpha) = E_1(\alpha) + E_2(\alpha) + E_3(\alpha) \tag{B12}$$

The development of this expression (B12) makes it possible to obtain the value of σ and α by the formula:

$$\frac{dE(\alpha_i)}{d\alpha_i} = 0 \tag{B13}$$

The expressions corresponding to $E_1(\alpha)$, $E_2(\alpha)$, and $E_3(\alpha)$, are:

$$E_1(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt\, u\left(s^2 - t^2\right) \times \left(\frac{\partial \Psi}{\partial s}\right)^2 \tag{B14}$$

$$E_2(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt\, u\left(s^2 - t^2\right) \times \left(\frac{\partial \Psi}{\partial t}\right)^2 \tag{B15}$$

$$E_3(\alpha) = -\int_0^\infty ds \int_0^s du \int_0^u dt \left[4Zsu - s^2 + t^2\right]\Psi^2 \tag{B16}$$

The normalization constant is as follows:

$$N = \int_0^\infty ds \int_0^s du \int_0^u dt\, u\left(s^2 - t^2\right) \times \Psi^2 \tag{B17}$$

With these changes of variables, we obtain the equations presented above in section (2.3): Equation (33; 34; 35).