

Calculation of Resonance Energies of $1,3P^0$, $1,3D^e$, $1,3F^0$, $1,3G^e$, $1,3H^0$ Doubly Excited States of Helium-Like Ions Systems Associated with $n = 2, 3$ and $n = 4$ Hydrogenic Thresholds Using the Hylleraas-Type Wave Functions

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Abstract

In this paper, the kinetic energy, the electrons-nucleus interaction energy, the electron-electron interaction energy and the total energy of doubly excited states of He-like ions are developed in the framework of the variational method using configuration interaction basis with a real Hamiltonian. Correlated Hylleraas-type wave functions are also used in this work in which several lower-lying doubly excited ($nl_1nl_2; l_1 \neq l_2$) $1,3P^0$, $1,3D^e$, $1,3F^0$, $1,3G^e$, $1,3H^0$ intrashell resonances associated with $n = 2, 3$ and 4 thresholds up to $Z = 10$ are reported. The results obtained are compared with some theoretical calculations of the available literature.

Keywords

Hylleraas Method, Helium-Like Ions Systems, Kinetic Energy, Electrons-Nucleus Interaction, Electron-Electron Interaction

1. Introduction

Doubly excited states (DES) of helium-like ions have been the subject of many studies by different physicists as the first seminal photoabsorption experiment realized by Madden and Codling [1] [2] and the theoretical explanation by Cooper *et al.* [3]. The doubly excited states of two-electron atoms are highly correlated states and they cannot be described in general like a simple model based on independent-particle quantum numbers. This experiment pushed theoreticians and

experimentalists to take an interest in the study of doubly excited states and particularly to the regime near the double ionization threshold, which represents a paradigm for electronic correlations in atomic physics.

Highly DES plays an important role in the ionization by low frequency intense laser pulses [4] [5], the understanding of collisional and radiational processes which take place in hot astrophysical and laboratory plasma [6] [7].

Over the years, a great effort has been made toward the investigation of electronic motions for the doubly excited resonances in helium atoms including model atoms, quantum dots systems, and natural two-electron systems, such as the helium atom. It's for this purpose that many theorists and many experimenters are interested in these resonances concerning the classification of the intrashell doubly excited states for two electron systems. These DES resonances have been investigated by Herrick and Sinanoglu [8] and Kellman and Herrick [9] and the underlying symmetries of two-electron Hamiltonian [9] [10].

As far as the excited states of helium-like ions are concerned, various methods of computations have been used. Among these methods, Oza [11] used the algebraic variational and a pseudostate close-coupling method to study resonances in He^+ ions below the $N=2$ threshold of the ion, Bhatia and Temkin used Feshbach projection formalism together with exchange scattering nonresonant continuum to calculate the width [12]. Seminario and Sanders [13] used a Feshbach projection Z -dependant perturbation method to investigate resonances in helium-like atoms sequence with $Z=2$ to 10. Calculations involving complex Hamiltonians or complex wave functions have also been used to calculate the $2s2p\ ^1P^0$ and $^3P^0$ resonances in He. Use of the complex rotation method in Z -dependant perturbation theory simultaneously yields values of the resonance position and width for the $2s2p\ ^1P^0$ autoionizing states of two-electron atoms to high order by Maning and Sanders [14]. A fully numerical multiconfiguration Hartree-Fock program has been modified for performance of calculations on atomic quasibound states using complex-coordinate technique by Bentley [15]. Using the complex-coordinate method, doubly excited states of helium sequence ($Z=1-10$) are investigated by Ho [16] and complex-coordinate rotation by the present authors [17]. Xi Wang *et al.* [18] have made an investigation on the doubly excited $^1P^0$ resonance states of helium atom in quantum plasmas using correlated exponential wave functions within the framework of the stabilization method.

The present work is an extension of the earlier calculations of two-photon excitation and ionization energies of the Rydberg helium [19].

In summary, our research is expanded toward DES intrashell states ($n_l n_b$) where both electrons occupy the same shell, and have high and equal values of the principal quantum number n . The electronic correlation effects may be as shown by Fano [20]. We employ special forms of the Hylleraas-type wave functions constructed without Slater type orbital and make use of the variational method combined to the configuration interaction states and a real Hamiltonian.

In Section 2, we present our wave functions, the analytical expression of kinetic

energy, electrons-nucleus interaction energy, electron-electron interaction energy and total energy for $(nl_1nl_2; l_1 \neq l_2) \ ^1P^0, \ ^1D^e, \ ^1F^0, \ ^1G^e, \ ^1H^0$ of doubly excited states of He-like ions.

In Section 3, the presentation and the discussion of our results in the case of doubly excited states $(2s2p) \ ^1P^0, (3s3p) \ ^1P^0, (3s3d) \ ^1D^e, (3p3d) \ ^1F^0, (4s4p) \ ^1P^0, (4s4d) \ ^1D^e, (4s4f) \ ^1F^0, (4p4d) \ ^1F^0, (4p4f) \ ^1G^e$ and $(4d4f) \ ^1H^0$ of helium-like ions up to $Z=10$ are made. Rydberg units are used throughout the present work. Some of our results are compared to available theoretical values. Here also, we have no experimental data and there is not much theoretical data available, for comparisons. Finally, we end with a conclusion.

2. Theoretical Method

2.1. Hamiltonian and Wave Functions

In our present work, the method of variational is used to calculate doubly excited intrashell resonance parameters of He-like ions. The interest of using this method is that resonance parameters can be obtained by using bound-state-type wave functions and no product of Slater-type orbitals are necessarily used. The Schrödinger equation for the relative motion of the helium-like ion, which interacts with each other by a spherically symmetric potential, can be written as:

$$H\Phi(\mathbf{r}_1, \mathbf{r}_2) = E\Phi(\mathbf{r}_1, \mathbf{r}_2), \quad (1)$$

When H is the non-relativistic Hamiltonian operator (in electron-volt) describing the three-body atomic system, with the nucleus being infinitely heavy, is given by:

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (2)$$

The vector \mathbf{r}_1 and \mathbf{r}_2 denote respectively the spatial coordinates of the electrons 1 and 2 from the nucleus, m the mass of an electron, e the elementary charge and Z the nuclear charge number, Δ_1 and Δ_2 are the Laplacian operators in position representation of the radius vectors \mathbf{r}_1 and \mathbf{r}_2 .

r_1 and r_2 are respectively used for $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$.

$$|\mathbf{r}_1 - \mathbf{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2 \cos \theta_{12}}$$

represente the relative distance between the two electrons.

θ_{12} : is the mutual angle between the position vectors of the electrons.

The Hamilton operator can be of three parts:

$$H = T + C + W, \quad (3)$$

where T , C and W are respectively the kinetic energy operator of the two electrons, the coulomb interaction operator between the atomic nucleus and the two electrons and the coulomb interaction operator between the two electrons:

$$T = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2), \quad (4)$$

$$C = -\frac{Ze^2}{r_1} - \frac{Ze^2}{r_2}, \quad (5)$$

$$W = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (6)$$

In this case of the Hamilton operator, all magnetic and relativistic effects together with the motion of the atomic nucleus are neglected.

In this article, $\Phi(\mathbf{r}_1, \mathbf{r}_2)$ are the trials non-orthogonal of two-electron wave functions that we have considered for the description of the intrashell singlet doubly excited states of the helium-like ions. There are special constructions of the incomplete hydrogenic wave functions and Hylleraas type wave functions as follows:

$$\Phi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2) = \chi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2) \varphi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2), \quad (7)$$

with

$$\varphi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2) = (r_1 + r_2)^j (r_1 - r_2)^k |\mathbf{r}_1 - \mathbf{r}_2|^m \exp[-\lambda(r_1 + r_2)], \quad (8)$$

which are Hylleraas ground state wave functions of the helium-like ions [21] [22], including electron correlation effects.

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;

and m : takes into account the distance between the two electrons.

j, k, m are also called Hylleraas parameters with ($j, k, m \geq 0$).

λ is the nonlinear variational parameter defined by:

$$\lambda = \frac{Z}{\alpha n a_0}, \quad (9)$$

where Z , α , a_0 and n are respectively the nucleus charge number, variational parameters, Bohr's radius and the principal quantum number.

These wave functions $\varphi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2)$ are not orthogonal.

The set of parameters (j, k, m) define the basis states (*i.e.* the configurations).

The even values of k define the symmetric wave functions describing the singlet states.

The wave functions $\Phi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2)$, are incomplete hydrogenic wave functions of the Hylleraas type for the doubly excited intrashell resonances and lower-lying states and can be expressed as follows:

$$\begin{aligned} \Phi_{n,l_1,l_2}(\mathbf{r}_1, \mathbf{r}_2) = & \left\{ (2r_1 2r_2)^{l_1} \sum_{\nu_1=0}^{\nu_1=n-l_1-1} \left[(n^2 a_0^2 \lambda^2) (2r_1 2r_2) \right]^{\nu_1} \right. \\ & \left. + (2r_1 2r_2)^{l_2} \sum_{\nu_2=0}^{\nu_2=n-l_2-1} \left[(n^2 a_0^2 \lambda^2) (2r_1 2r_2) \right]^{\nu_2} \right\} \\ & \times (r_1 + r_2)^j (r_1 - r_2)^k \times |\mathbf{r}_1 - \mathbf{r}_2|^m \exp[-\lambda(r_1 + r_2)], \end{aligned} \quad (10)$$

with

$n = (j, k, m)$ is the principal quantum number of the two electrons;

l_1 and l_2 are orbital angular momentum for the two electrons.

The interesting feature in the wave functions $\Phi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2)$, is that they contain an electron correlation term: $|\mathbf{r}_1 - \mathbf{r}_2|$, which represents the angular part of the wave functions instead of the spherical harmonic in the other Hylleraas type wave functions.

This electron correlation term plays an important role in our trial wave functions for the description of the intrashell singlet doubly excited states. The wave functions $\Phi_{j,k,m}(\mathbf{r}_1, \mathbf{r}_2)$ have also the advantage that, in the eigenvalue calculations E , the exhibition of a plateau and the convergence of the minima of the functions ($dE/d\alpha = 0$) arise quickly for small basis set (13 terms).

2.2. Calculation Procedures

The final form of the wave functions of the intrashell singlet doubly excited state including the correlation effects due to the mixing of configurations can be expressed as follows:

$$\psi_{n,l_1,l_2}(\mathbf{r}_1, \mathbf{r}_2) = \sum_n a_n \Phi_{n,l_1,l_2}, \tag{11}$$

where a_n are the eigenvectors which can be determined by solving the Schrödinger equation.

$$H\psi_{n,l_1,l_2}(\mathbf{r}_1, \mathbf{r}_2) = E\psi_{n,l_1,l_2}(\mathbf{r}_1, \mathbf{r}_2), \tag{12}$$

The representation of the Schrodinger equation on the non-orthogonal basis leads to the general eigenvalue equation:

$$\sum_n (H_{n,n} - EN_{n,n})a_n = 0, \tag{13}$$

with:

$$N_{n,n} = N_{J,K,M} = \langle \psi_{n,l_1,l_2} | \psi_{n,l_1,l_2} \rangle, \tag{14}$$

$$H_{n,n} = H_{J,K,M} = \langle \psi_{n,l_1,l_2} | H | \psi_{n,l_1,l_2} \rangle, \tag{15}$$

$$H_{n,n} = H_{J,K,M} = \langle \psi_{n,l_1,l_2} | T + C + W | \psi_{n,l_1,l_2} \rangle, \tag{16}$$

$$H_{n,n} = \langle \psi_{n,l_1,l_2} | T | \psi_{n,l_1,l_2} \rangle + \langle \psi_{n,l_1,l_2} | C | \psi_{n,l_1,l_2} \rangle + \langle \psi_{n,l_1,l_2} | W | \psi_{n,l_1,l_2} \rangle, \tag{17}$$

$$T_{n,n} = T_{J,K,M} = \langle \psi_{n,l_1,l_2} | T | \psi_{n,l_1,l_2} \rangle = T, \tag{18}$$

$$C_{n,n} = C_{J,K,M} = \langle \psi_{n,l_1,l_2} | C | \psi_{n,l_1,l_2} \rangle = C, \tag{19}$$

$$W_{n,n} = W_{J,K,M} = \langle \psi_{n,l_1,l_2} | W | \psi_{n,l_1,l_2} \rangle = W, \tag{20}$$

$$H_{J,K,M} = T_{J,K,M} + C_{J,K,M} + W_{J,K,M} = E = T + C + W, \tag{21}$$

wherein $N_{J,K,M}$ are the matrix elements of normalisation factor, $H_{J,K,M}$ the matrix elements of Hamilton operator, $T_{J,K,M}$ the matrix elements of kinetic energy operator of the two electrons, $C_{J,K,M}$ the matrix elements of electrons-nucleus interaction energy operator and $W_{J,K,M}$ the matrix elements of electron-electron interaction energy operator.

For example, we present the result of the different parameters of $2s2p^1P^0$ state:

- Matrix elements of normalization factor:

$$\begin{aligned}
 N_{J,K,M} = & \frac{2\pi^2}{M+2} \left(\frac{1}{K+1} - \frac{1}{K+3} - \frac{1}{K+M+3} + \frac{1}{K+M+5} \right) (J+K+M+5)! \left(\frac{1}{2\lambda} \right)^{J+K+M+6} \\
 & + \frac{4\pi^2}{M+2} (1+n^2 a_0^2 \lambda^2) \left(\frac{1}{K+1} - \frac{2}{K+3} + \frac{1}{K+5} - \frac{1}{K+M+3} + \frac{2}{K+M+5} \right. \\
 & \left. - \frac{1}{K+M+7} \right) (J+K+M+7)! \left(\frac{1}{2\lambda} \right)^{J+K+M+8} \\
 & + \frac{2\pi^2}{M+2} (1+n^2 a_0^2 \lambda^2)^2 \left(\frac{1}{K+1} - \frac{3}{K+3} + \frac{3}{K+5} - \frac{1}{K+7} - \frac{1}{K+M+3} \right. \\
 & \left. + \frac{3}{K+M+5} - \frac{3}{K+M+7} + \frac{1}{K+M+9} \right) (J+K+M+9)! \left(\frac{1}{2\lambda} \right)^{J+K+M+10} \quad (22)
 \end{aligned}$$

for $K = 0, 2, 4, 6, \dots$

$$N_{J,K,M} = 0 \text{ for } K = 1, 3, 5, 7, \dots$$

- Matrix elements of electrons-nucleus interaction energy:

$$\begin{aligned}
 C_{J,K,M} = & \frac{2\pi^2}{M+2} \left(\frac{1}{K+1} - \frac{1}{K+M+3} \right) (J+K+M+4)! \left(\frac{1}{2\lambda} \right)^{J+K+M+5} \\
 & + \frac{16\pi^2}{M+2} (1+n^2 a_0^2 \lambda^2) \left(\frac{1}{K+1} - \frac{1}{K+3} - \frac{1}{K+M+3} + \frac{1}{K+M+5} \right) \\
 & \times (J+K+M+6)! \left(\frac{1}{2\lambda} \right)^{J+K+M+7} \\
 & + \frac{8\pi^2}{M+2} (1+n^2 a_0^2 \lambda^2)^2 \left(\frac{1}{K+1} - \frac{2}{K+3} + \frac{1}{K+5} - \frac{1}{K+M+3} \right. \\
 & \left. + \frac{2}{K+M+5} - \frac{1}{K+M+7} \right) (J+K+M+8)! \left(\frac{1}{2\lambda} \right)^{J+K+M+9} \quad (23)
 \end{aligned}$$

for $K = 0, 2, 4, 6, \dots$

$$C_{J,K,M} = 0 \text{ for } K = 1, 3, 5, 7, \dots$$

- Matrix elements of electron-electron interaction energy:

$$W_{J,K,M} = e^2 N_{J,K,M-1} \quad (24)$$

- Matrix elements of kinetic energy:

$$\begin{aligned}
 T_{J,K,M} = & 2 \left(\lambda^2 N_{J,K,M} - J\lambda N_{J-1,K,M} + jj' N_{J-2,K,M} + kk' N_{J,K-2,M} + mm' N_{J,K,M-2} \right) \\
 & + \frac{1}{2} \left[-M\lambda (C_{J,K,M} - C_{J,K+2,M-2}) + (mj' + jm') (C_{J-1,K,M} - C_{J-1,K+2,M-2}) \right. \\
 & \left. + (mk' + km') (C_{J+1,K,M-2} - C_{J-1,K,M}) \right] \quad (25)
 \end{aligned}$$

All the other states are calculated with this same way.

The intrashell singlet doubly excited wave functions were found in the basics containing the configurations with the following condition for the Hylleraas parameters $j + k + m \leq 3$, corresponding to the basis dimension $D = 13$.

In order to obtain the minimum eigenvalue in which we are interested in the calculations are carried out for various values of the parameter α .

The eigenvalues E obtained in the present calculations follow the Hylleraas-Undheim theorem [23] and do not include the Feshbach shifts because of the use of the incomplete basis sets of the wave functions.

According to the Hylleraas-Undheim theorem [23], a good approximation for the eigenvalues is obtained when the minima of the functions ($dE/d\alpha = 0$) converge with increasing values of the dimension D and when the functions exhibit a plateau.

In our approach, for example to calculate the resonance parameters of the $2s2p\ ^1P^0$ state, we fix the variational parameter α and determine each time the value of the energy E . In **Table 1**, we notice that E varies slowly but we clearly see that it decreases until $\alpha = 1.1$ and corresponds to $E = -1.410176$ Ry.

Table 1. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(2s2p)\ ^1P^0$ state of helium-like ions ($Z = 2$) depending on the variational parameter α . The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV.

α	0.300000	0.400000	0.500000	0.600000	0.700000	0.800000
T	5.755883	3.395141	2.342141	1.820539	1.564662	1.455149
C	-6.425211	-4.996593	-4.195378	-3.728785	-3.472319	-3.353518
W	1.063901	0.796690	0.648398	0.562257	0.514444	0.491661
E	0.394573	-0.804761	-1.204838	-1.345988	-1.393212	-1.406707
α	0.900000	1.000000	1.100000	1.200000	1.300000	1.400000
T	1.419468	1.411248	1.409646	1.409165	1.408162	1.405059
C	-3.312497	-3.302572	-3.300631	-3.300172	-3.299166	-3.295751
W	0.483339	0.481167	0.480808	0.480879	0.480956	0.480839
E	-1.409689	-1.410156	-1.410176	-1.410128	-1.410047	-1.409851
α	1.500000	1.600000	1.700000	1.800000	1.900000	2.000000
T	1.398312	1.386401	1.367742	1.341044	1.305881	1.262946
C	-3.288149	-3.274537	-3.252820	-3.221030	-3.178098	-3.124316
W	0.480461	0.479738	0.478416	0.476102	0.472428	0.467199
E	-1.409374	-1.408397	-1.406661	-1.403882	-1.399788	-1.394169

3. Results and Discussions

In **Tables 2-11**, we show the variation, of the kinetic energies T , the electrons-nucleus interaction energies C , the electron-electron interaction energies W and the total energies E of the present work for $(2s2p)\ ^1,^3P^0$, $(3s3p)\ ^1,^3P^0$, $(3s3d)\ ^1,^3D^e$, $(3p3d)\ ^1,^3F^0$, $(4s4p)\ ^1,^3P^0$, $(4s4d)\ ^1,^3D^e$, $(4s4f)\ ^1,^3F^0$, $(4p4d)\ ^1,^3F^0$ $(4p4f)\ ^1,^3G^e$ and $(4d4f)\ ^1,^3H^0$ states of helium-like ions with $Z = 2 - 10$.

Table 2. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(2s2p) \ ^1P^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

Z	2	3	4	5	6	7	8	9	10
$2s2p \ ^1P^0$									
T	1.409646	3.556518	6.698735	10.842019	15.981076	22.119677	29.257977	37.396075	46.534037
C	-3.300631	-7.931851	-14.564477	-23.201567	-33.836143	-46.471498	-61.107384	-77.743657	-96.380231
W	0.480808	0.818336	1.166202	1.519452	1.875488	2.233405	2.592559	2.952567	3.313191
E	-1.410176	-3.556996	-6.699540	-10.840095	-15.979578	-22.118415	-29.256847	-37.395014	-46.533002
$2s2p \ ^3P^0$									
T	1.551046	3.798303	7.045029	11.291638	16.538180	22.784692	30.031200	38.277715	47.524248
C	-3.495628	-8.240897	-14.986652	-23.732740	-34.479017	-47.225433	-61.971965	-78.718599	-97.465329
W	0.393482	0.644273	0.896495	1.149354	1.402548	1.655939	1.909457	2.163060	2.416724
H	-1.551099	-3.798320	-7.045127	-11.291747	-16.538289	-22.784801	-30.031307	-38.277823	-47.524356

Table 3. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(3s3p) \ ^1P^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

Z	2	3	4	5	6	7	8	9	10
$3s3p \ ^1P^0$									
T	0.721806	1.743063	3.185168	5.168438	7.509442	10.285995	13.498918	17.148572	21.235117
C	-1.629587	-3.791826	-6.816640	-10.828300	-15.640876	-21.333656	-27.907474	-35.362619	-43.699167
W	0.238319	0.391043	0.546509	0.706628	0.867911	1.031050	1.195586	1.361175	1.527570
H	-0.669461	-1.657720	-3.084962	-4.953233	-7.263522	-10.016610	-13.212969	-16.852870	-20.936479
$3s3p \ ^3P^0$									
T	0.768403	1.803668	3.344628	5.328445	7.625119	10.415003	13.638987	17.297331	21.390157
C	-1.688254	-3.863953	-6.991190	-10.998171	-15.768679	-21.472579	-28.054519	-35.514806	-43.853579
W	0.208538	0.332778	0.461361	0.588854	0.713286	0.839675	0.966275	1.093033	1.219908
H	-0.711312	-1.727506	-3.185201	-5.080871	-7.430273	-10.217900	-13.449255	-17.124441	-21.243513

Table 4. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(3s3d) \ ^1D^e$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

Z	2	3	4	5	6	7	8	9	10
$3s3d \ ^1D^e$									
T	0.656972	1.676123	3.136619	5.107558	7.437827	10.203242	13.405236	17.044199	21.120237
C	-1.509119	-3.683365	-6.739832	-10.738866	-15.536950	-21.214396	-27.773039	-35.213267	-43.535106
W	0.213194	0.377033	0.538811	0.699589	0.861030	1.024251	1.188866	1.354536	1.521008
H	-0.638952	-1.630209	-3.064401	-4.931718	-7.238091	-9.986902	-13.178936	-16.814531	-20.893860
$3s3d \ ^3D^e$									
T	0.699180	1.785066	3.297155	5.217635	7.566095	10.347461	13.562951	17.212907	21.297440
C	-1.568557	-3.814243	-6.920876	-10.867519	-15.683227	-21.375170	-27.945079	-35.393429	-43.720363
W	0.189600	0.326302	0.456298	0.582864	0.709178	0.835670	0.962348	1.089171	1.216102
H	-0.679776	-1.702875	-3.167422	-5.067019	-7.407954	-10.192038	-13.419779	-17.091349	-21.206820

Table 5. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(3p3d) \ ^1\text{F}^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$3p3d \ ^1\text{F}^0$										
T		0.629939	1.583288	2.979055	4.812629	7.089337	9.809586	12.973643	16.581685	20.633831
C		-1.469297	-3.516557	-6.456078	-10.280301	-14.994157	-20.597486	-27.090173	-34.472128	-42.743282
W		0.207525	0.349296	0.500465	0.656654	0.816564	0.979056	1.143405	1.309130	1.475898
H		-0.631832	-1.583972	-2.976557	-4.811017	-7.088255	-9.808843	-12.973123	-16.581312	-20.633551
$3p3d \ ^3\text{F}^0$										
T		0.671387	1.656249	3.083758	4.958420	7.274220	10.034445	13.239097	16.888183	20.981710
C		-1.529178	-3.618737	-6.599089	-10.472152	-15.231182	-20.879443	-27.416816	-34.843238	-43.158672
W		0.184954	0.306024	0.430922	0.557411	0.684538	0.812194	0.940195	1.068431	1.196837
H		-0.672837	-1.656464	-3.084407	-4.956320	-7.272424	-10.032803	-13.237523	-16.886622	-20.980124

Table 6. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4s4p) \ ^1\text{P}^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$4s4p \ ^1\text{P}^0$										
T		0.382227	0.946782	1.750000	2.800205	4.098185	5.644330	7.438817	9.481716	11.773049
C		-0.875729	-2.065196	-3.744224	-5.921253	-8.597080	-11.771979	-15.445986	-19.619041	-24.291050
W		0.123072	0.200570	0.282260	0.367234	0.454818	0.544460	0.635731	0.728300	0.821914
H		-0.370430	-0.917843	-1.711962	-2.753813	-4.044076	-5.583188	-7.371438	-9.409024	-11.696086
$4s4p \ ^3\text{P}^0$										
T		0.404489	0.967613	1.773480	2.866925	4.181971	5.745029	7.556065	9.615036	11.921905
C		-0.903688	-2.096307	-3.782376	-6.007075	-8.703991	-11.899234	-15.592654	-19.784134	-24.473587
W		0.112622	0.183071	0.255860	0.330398	0.405921	0.482096	0.558718	0.635659	0.712831
H		-0.386576	-0.945622	-1.753035	-2.809751	-4.116099	-5.672108	-7.477870	-9.533439	-11.838849

Table 7. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4s4d) \ ^1\text{D}^e$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$4s4d \ ^1\text{D}^e$										
T		0.378690	0.935032	1.740104	2.790332	4.087033	5.631502	7.424205	9.465291	11.754807
C		-0.866906	-2.048387	-3.730073	-5.907102	-8.581152	-11.753745	-15.425303	-19.595870	-24.265385
W		0.120289	0.198552	0.280931	0.366140	0.453767	0.543411	0.634677	0.727241	0.820851
H		-0.367926	-0.914802	-1.709037	-2.750629	-4.040351	-5.578830	-7.366420	-9.403337	-11.689727
$4s4d \ ^3\text{D}^e$										
T		0.393815	0.956434	1.790212	2.857389	4.171413	5.733097	7.542654	9.600113	11.905458
C		-0.887971	-2.080239	-3.795150	-5.993688	-8.689163	-11.882497	-15.573870	-19.763257	-24.450599
W		0.110205	0.181337	0.254793	0.329543	0.405129	0.481329	0.557965	0.634915	0.712095
H		-0.383950	-0.942467	-1.750144	-2.806755	-4.112620	-5.668070	-7.473249	-9.528228	-11.833045

Table 8. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4s4f) \ ^1F^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$4s4f \ ^1F^0$										
T		0.360118	0.923018	1.739458	2.780225	4.076135	5.618920	7.409806	9.449062	11.736750
C		-0.833461	-2.020785	-3.721165	-5.892338	-8.565492	-11.735817	-15.404895	-19.572955	-24.239965
W		0.114007	0.193102	0.277955	0.365006	0.452738	0.542382	0.633638	0.726194	0.819800
H		-0.359335	-0.904664	-1.703750	-2.747106	-4.036619	-5.574514	-7.361450	-9.397698	-11.683414
$4s4f \ ^3F^0$										
T		0.375815	0.949770	1.776567	2.849558	4.162967	5.723109	7.530997	9.586784	11.890474
C		-0.855111	-2.058308	-3.774791	-5.982080	-8.676859	-11.868116	-15.557213	-19.744312	-24.429384
W		0.104342	0.176538	0.253193	0.328784	0.404453	0.480653	0.557283	0.634228	0.711405
H		-0.374953	-0.931999	-1.745030	-2.803737	-4.109437	-5.664353	-7.468933	-9.523299	-11.827503

Table 9. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4p4d) \ ^1F^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$4p4d \ ^1F^0$										
T		0.377564	0.931412	1.731863	2.779309	4.074296	5.617245	7.408402	9.447886	11.735752
C		-0.864954	-2.042848	-3.718223	-5.891501	-8.563214	-11.733712	-15.403133	-19.571486	-24.238724
W		0.119979	0.197904	0.279823	0.364929	0.452580	0.542256	0.633545	0.726125	0.819746
H		-0.367410	-0.913531	-1.706535	-2.747261	-4.036337	-5.574209	-7.361185	-9.397474	-11.683225
$4p4d \ ^3F^0$										
T		0.392623	0.953248	1.782548	2.847358	4.159928	5.720312	7.528542	9.584624	11.888552
C		-0.885930	-2.075279	-3.784310	-5.979674	-8.673157	-11.864684	-15.554207	-19.741677	-24.427046
W		0.109914	0.180821	0.253942	0.328651	0.404275	0.480512	0.557176	0.634146	0.711341
H		-0.383392	-0.941210	-1.747819	-2.803664	-4.108953	-5.663859	-7.468488	-9.522906	-11.827153

Table 10. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4p4f) \ ^1G^e$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

	Z	2	3	4	5	6	7	8	9	10
$4p4f \ ^1G^e$										
T		0.361420	0.917805	1.728398	2.767067	4.062856	5.604830	7.394425	9.432152	11.718194
C		-0.835491	-2.014723	-3.705335	-5.873392	-8.546556	-11.715846	-15.383184	-19.549156	-24.213909
W		0.114311	0.192470	0.276560	0.363548	0.451491	0.541235	0.632533	0.725107	0.818721
E		-0.359759	-0.904447	-1.700376	-2.742776	-4.032208	-5.569780	-7.356224	-9.391896	-11.676993
$4p4f \ ^3G^e$										
T		0.377083	0.944754	1.765231	2.836166	4.149753	5.709380	7.516280	9.570844	11.873193
C		-0.857059	-2.052467	-3.758744	-5.963291	-8.658429	-11.849018	-15.536761	-19.722167	-24.405376
W		0.104606	0.175948	0.251961	0.327613	0.403489	0.479792	0.556474	0.633448	0.710644
E		-0.375369	-0.931764	-1.741551	-2.799512	-4.105187	-5.659845	-7.464006	-9.517873	-11.821538

Table 11. Kinetic energies T , the electron-nucleus energies C , the electron-electron energies W and the total energies E of $(4d4f) \ ^1H^0$ state of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: $1 \text{ Ry} = 13.6056925 \text{ eV}$.

Z	2	3	4	5	6	7	8	9	10
$4d4f \ ^1H^0$									
T	0.363752	0.913058	1.711677	2.763292	4.063333	5.611884	7.409275	9.455792	11.751644
C	-0.839208	-2.008834	-3.681602	-5.858547	-8.534613	-11.709765	-15.384300	-19.558471	-24.232439
W	0.114866	0.192091	0.274470	0.359654	0.447211	0.536694	0.627752	0.720101	0.813511
E	-0.360588	-0.903683	-1.695454	-2.735600	-4.024068	-5.561185	-7.347272	-9.382578	-11.667283
$4d4f \ ^3H^0$									
T	0.378224	0.939796	1.749296	2.813019	4.124580	5.683574	7.490021	9.544009	11.845612
C	-0.859352	-2.046876	-3.736228	-5.930864	-8.623454	-11.813381	-15.500651	-19.685368	-24.367622
W	0.104930	0.175942	0.250210	0.325565	0.401632	0.478163	0.555027	0.632136	0.709432
E	-0.376197	-0.931137	-1.736720	-2.792278	-4.097241	-5.651643	-7.455602	-9.509222	-11.812576

Table 12 and **Table 13** contain comparison electron-electron interaction energies W of the present work with results of Sakho *et al.* have used the Screening Constant by Unit Nuclear Charge (SCUNC) method [24] [25], and Ivanov and Safronova, have used the method of computing double sums over the complete hydrogen spectrum [26] for $(2s2p) \ ^1P^0$ and $(3s3p) \ ^1P^0$ states of helium-like ions ($Z = 2 - 10$). Electron-electron correlation is essential for the process of excitation and ionization and is great when the nucleus charge number Z increase. In these cases, we did not find any experimental results for comparison.

Table 12. Comparison of the calculations of electron-electron energies W of the $(2s2p) \ ^1P^0$ state of helium-like ions ($Z = 2 - 10$) with results from other authors.

Z	2	3	4	5	6	7	8	9	10
$2s2p \ ^1P^0$									
W^a	0.480808	0.818336	1.166202	1.519452	1.875488	2.233405	2.592559	2.952567	3.313191
W^b	0.612243	0.989291	1.367074	1.744122	2.121905	2.498953	2.876735	3.253783	3.631566
W^c	0.572554	0.955482	1.338409	1.720602	2.103530	2.486458	2.869386	3.252313	3.635241

^aPresent work, ^bI. Sakho *et al.* [24] [25], ^cA. I. Ivanov, I. U. Safronova [26].

Table 13. Comparison of the calculations of electron-electron energies W of the $(3s3p) \ ^1P^0$ state of helium-like ions ($Z = 2 - 10$) with results from other authors.

Z	2	3	4	5	6	7	8	9	10
$3s3p \ ^1P^0$									
W^a	0.238319	0.391043	0.546509	0.706628	0.867911	1.031050	1.195586	1.361175	1.527570
W^b	0.219760	0.348383	0.477006	0.605628	0.734251	0.862873	0.991496	1.120118	1.249476
W^c	0.280029	0.445401	0.611508	0.777615	0.942987	1.109094	1.274466	1.440572	1.606679

^aPresent work, ^bI. Sakho *et al.* [24] [25], ^cA. I. Ivanov, I. U. Safronova [26].

In **Table 12**, we note a difference between our results and those of Sakho *et al.* and Ivanov and al. In **Table 13**, our results are much closer to those of Ivanov *et al.* than those of Sakho *et al.* In these two tables, the difference in behavior can be explained by the interactions created by the significant presence of the nuclear charge.

We compared the **Table 14** and **Table 15**, to our results of the total energies E for $(2s2p) \ ^1\text{P}^0$ and $(3s3p) \ ^1\text{P}^0$ the states of helium-like ions ($Z = 2 - 10$) with the theoretical values of Ho. [16], Drake and Delgarno [27], Seminario and Sanders [13], Sakho *et al.* [24] [25], and Bachau *et al.* [28] which have respectively used the complex-coordinate method, the energy maximization method, the Feshbach projection method, the Screening Constant by Unit Nuclear Charge (SCUNC) method, the pseudo-potential-Feshbach method (PPF) with the character of the closed-channel wave function. Comparison shows a good agreement between the present calculations and theoretical results of these authors. The disagreements noted between our results and those of the other calculations can be explained by the fact that we neglected in the present calculations the Feshbach shifts. These disagreements can also be explained by the choice of the angular part of the wave functions used for the description of the doubly excited states of the helium like-ions.

Table 14. Comparison of the calculations of energies E of the $(2s2p) \ ^1\text{P}^0$ state of helium-like ions ($Z = 2 - 10$) with results from other authors.

	Z	2	3	4	5	6	7	8	9	10
$2s2p \ ^1\text{P}^0$										
$-E^a$		1.410176	3.556996	6.699540	10.840095	15.979578	22.118415	29.256847	37.395014	46.533002
$-E^b$		1.38627	3.51512	6.63896	10.76042	15.88056	21.99993	29.11878	37.23735	46.35555
$-E^c$		1.38708	3.51526	6.64030	10.76186	15.88206	22.00146	29.12034	37.23886	46.35712
$-E^d$		1.38508	3.51402	6.63778	10.75916	15.87924	21.99854	29.11734	37.23574	46.35394
$-E^e$		1.38875	3.51124	6.63574	10.75592	15.88274	22.00624	29.12974	37.25324	46.37670
$2s2p \ ^3\text{P}^0$										
$-E^a$		1.551099	3.798320	7.045127	11.291747	16.538289	22.784801	30.031307	38.277823	47.524356
$-E^b$		1.52099	3.75637	6.99127	11.22598	16.46057	22.69511	29.92561	38.16408	47.39853
$-E^c$		1.52114	3.75650	6.99140	11.22610	16.46069	22.69522	29.92972	38.16419	47.39862
$-E^d$		1.52294	3.75877	6.99391	11.22875	16.46345	22.69805	29.93260	38.16705	47.40155
$-E^e$		1.52765	3.75406	6.68046	11.20686	16.43326	22.36966	29.88606	38.11246	47.33886

^aPresent work, ^bHo [16], ^cDrake and dalgarno [27], ^dSeminario and sanders [13], ^eSakho *et al.* [24] [25].

Table 15. Comparison of the calculations of energies E of the $(3s3p) \ ^1\text{P}^0$ state of helium-like ions ($Z = 2 - 10$) with results from other authors.

	Z	2	3	4	5	6	7	8	9	10
$3s3p \ ^1\text{P}^0$										
$-E^a$		0.669461	1.65772	3.084962	4.953233	7.263522	10.01661	13.212969	16.85287	20.936479
$-E^b$		0.67125	1.65760	3.08770	4.96180	7.28050	10.04350	13.25100	16.90280	20.99900

Continued

$-E^c$	0.67140	1.65940	3.09000	4.96600	7.28600	10.04800	13.25600	16.91000	21.00000
$-E^d$	0.66884	1.65151	3.07812	4.94939	7.26533	10.02521	13.23048	16.87969	20.97283
$3s3p\ ^3P^0$									
$-E^a$	0.711312	1.727506	3.185201	5.080871	7.430273	10.217900	13.449255	17.124441	21.243513
$-E^b$	0.70080	1.71010	3.16390	5.06210	7.40480	10.19190	13.42350	17.09950	21.22000
$-E^e$	0.70360	1.71380	3.16390	5.06210	7.40480	10.19190	13.42350	17.09950	21.22000

^aPresent work, ^bHo [16], ^cBachau *et al.* [28], ^dSakho *et al.* [24] [25].

Kinetic energy is the first term of the Hamiltonian, which defines the total energy of system. The interest in calculating the kinetic energy of electrons lies the equilibrium and stability of matter, as stipulated by the virial theorem. It balances the attractive potential energy of the nucleus and prevents the electron from colliding with it. This calculation is central to the design of new materials and advanced quantum technologies such as superconductivity, semiconductors and nanotechnology.

The coulomb interaction is an essential attractive force between the positive charge of the nucleus (proton) and the negative charge of electron, representing the cohesive force of the atom. It is defined in a potential «well» where the electron is trapped and partially counteracts the attraction of the nucleus. This energy becomes negative and significant as the electron moves closer to the nucleus, which explains its strong bound. To identify chemical elements using spectroscopy, it is necessary to study the transitions of electrons between the different levels of coulomb interaction. Understanding these interactions allows us to design powerful lasers, explore imaging or radiotherapy techniques and plasma phenomena.

The coulomb interaction energy between electrons represents the repulsive electrostatic force that electrons exert on each other within an atom. This positive energy destabilizes the atom pushing electrons apart. This study is part of one of the most complex and important challenges in modern physics, especially in the design of materials at the atomic scale. The stable state of atom is the precise point where the total energy is minimal. This work provides theorists and experimentalists in the field of atomic and nuclear physics with a database for their different branches of research.

4. Conclusion

We have presented this paper, independently, using special forms of Hylleraas-type wave functions, the kinetic energies, the electrons-nucleus interaction energies, the electron-electron interaction energies and the total energies for $(2s2p)\ ^1,^3P^0$, $(3s3p)\ ^1,^3P^0$, $(3s3d)\ ^1,^3D^e$, $(3p3d)\ ^1,^3F^0$, $(4s4p)\ ^1,^3P^0$, $(4s4d)\ ^1,^3D^e$, $(4s4f)\ ^1,^3F^0$, $(4p4d)\ ^1,^3F^0$, $(4p4f)\ ^1,^3G^e$ and $(4d4f)\ ^1,^3H^0$ resonance states for He-like ions below the $n = 2, 3$ and 4 hydrogenic thresholds up to $Z = 10$. The calculations have been done in the framework of the variation method using configuration interaction basis states with a real Hamiltonian. Our results for total energies are in good

agreement with cited theoretical literatures values and other methods. For the electron-electron interaction energies, we have noted a slight disagreement between our results and those of the other calculations. In a general way, we have presented in this paper satisfactory results of some singlet doubly excited states of two-electron atoms for $n_1l_1n_2l_2$ ($l_1 \neq l_2$). The calculation of these different parameters will allow the community working in the field of atomic physics to understand the resonance phenomena linked to three-body atomic systems. Our future project is to predict the theoretical calculations for non-relativistic theories of singlet and triplet doubly excited resonances states $n_1l_1n_2l_2$ ($n_1 \neq n_2, l_1 \neq l_2$).

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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