Calculations Energy of the \((nl^2) \, ^1L_\pi\) Doubly Excited States of Two-Electron Systems via the Screening Constant by Unit Nuclear Charge Formalism

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Abstract

In this work, the total energies of doubly excited states \((ns^2) \, ^1S\), \((np^2) \, ^1D\), \((nf^2) \, ^1G\), \((nd^2) \, ^1I\), \((ng^2) \, ^1K\), and \((nh^2) \, ^1M\) of the helium iso-electronic sequence with \(Z \leq 10\) are calculated in the framework of the variational method of the Screening Constant by Unit Nuclear Charge Formalism. These calculations are performed using a new wavefunction correlated to Hylleraas-type. The possibility of using the SCUNC method in the investigation of high-lying Doubly Excited States (DES) in two-electron systems is demonstrated in the present work in the case of the \((nl^2) \, ^1L_\pi\) doubly excited states, where accurate total energies are tabulated up to \(n = 20\). All the results obtained in this paper are in agreement with the values of the available literature and may be useful for future experimental and theoretical studies on the doubly excited \((nl^2) \, ^1L_\pi\) states of two-electron systems.

Keywords

Doubly Excited States, Helium-Like Systems, Screening Constant by Unit Nuclear Charge (SCUNC), Wave Functions Correlated, Total Energy

1. Introduction

Studies of doubly-excited states of helium-like systems remain an active field of research since the early experiments of Madden and Codling [1] [2] concerning the observation of resonant structures in the absorption spectrum of helium using synchrotron radiation. The strong correlation between electrons in the
A doubly excited state of two-electron atomic systems has attracted considerable attention from theorists and experimenters as evidenced by the efforts concentrated in the field over the last twenty years. Theoretical investigations in two-electron Doubly Excited States (DES) are of great interest in connection with the understanding of collisional and radiative processes which take place in hot astrophysical and laboratory plasma [3] [4] [5]. In these investigations, great attention has been paid to the study of symmetric \((n\ell)\) DES where the electron-electron correlation effects may be predominant as revealed by the works of Fano [6]. Several experimental and theoretical studies on doubly excited \((n\ell)\) states have been carried out using different methods. Experimentally, many of these doubly excited states have been observed in electronic impact experiments by Oda et al. [7] and Hicks and Comer [8]. In their studies, these authors have worked on the energy spectra of ejected electrons from autoionization states in helium excited by electron impact. Other doubly excited states were observed by ion impact by Rudd [9] and by Bordenave-Montesquieu et al. [10]. These doubly excited states were also studied by examining the spectra of ejected electrons by Gelabart et al. [11] and by Rodbro et al. [12]. From a theoretical point of view, several calculation methods have been used, the complex rotation method [13] [14] [15], the variational method of Hylleraas [16], the double sums over the total hydrogen spectrum formalism [17], the density functional theory [18], the formalism of the Feshbach projection operators [19] [20], the discretization technique [21], the truncated diagonalization method [22], the time-dependent variation perturbation theory [23], and the semi-empirical procedure of the screening constant by unit nuclear charge (SCUNC) method [24] [25] [26], to name a few. In all these \(ab-initio\) methods, energies of \((nl2)\) 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. But, it’s widely believed that there are distinct advantages to viewing problems of physics within the framework of simple analytical models. Contrary to all these methods, the variational procedure of the SCUNC method makes it possible to calculate the energies of the \((n\ell)\) doubly excited states without a complex mathematical program or calculation code but from a simple analytical expression. In addition, in the recent past the variational procedure of the SCUNC method has been successfully applied to calculations of the energies of doubly excited states \(nlnl'\) \((n = 2 - 4)\) in helium-like ions by Sakho [27] using a special Hylleraas-type wave function. These reasons sufficiently justify our choice to apply the variational procedure of the SCUNC method in this study. The goal of the present work is to report accurate total energies and excitation energies of the doubly excited states \((n\ell)\) using the variational procedure of the SCUNC formalism but also to show that it is possible to calculate total energies and precise excitation energies of high-lying up to \(n = 20\) of the doubly excited states \((n\ell)\) without any calculation code or complex mathematical program, without a powerful computer but using a sim-
ple analytical expression. Section 2 gives the correlated wave functions and brief overview of the calculation method. Section 3 gives the presentation and the discussion of our results in the case of doubly excited states \((ns^2)^1S^\ell, (np^2)^1D^\ell, (nf^2)^1G^\ell, (ng^2)^1H^\ell, (nh^2)^1I^\ell,\) and \((nh^2)^1M^\ell\) of the He-like ions up to \(Z = 10\) are made. All our results are compared to available theoretical and experimental data.

2. Theory and Calculations

2.1. Hamiltonian and Hylleraas-Type Wave Functions

The time independent Schrödinger equation for the Helium atom, or the positive ions of its isoelectronic sequence, or of the negative Hydrogen ion, is

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

where \(\hat{H}\) represents the Hamiltonian operator of the considered system, \(\Psi\) the trial wave function and \(E\) the associated energy.

The Hamiltonian \(H\) of the helium isoelectronic series is given by (in atomic units)

\[
H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}
\]

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

Solving Equation (1) is very difficult because of the term \(r_{12}\) representing electron-electron repulsion. It is therefore necessary to implement a rough calculation method using a correlated wavefunction.

The groundbreaking work in this area was conducted by Hylleraas [28] [29] [30]. The simplest Hylleraas wave function is written as follow:

\[
\Psi(r_1, r_2, r_{12}) = (1 + br_{12}) \exp[-\alpha(r_1 + r_2)]
\]

Since Hylleraas’ original work, tremendous efforts have been made to improve upon that work, using larger and larger expansions, adding more complicated terms. In this present work, we have modified this Hylleraas wavefunction in order to adapt it to the study of symmetrical \((n\ell^2)^1L^\ell\) doubly excited states in two-electron atomic systems. These wave functions are defined as follow:

\[
\Psi(r_1, r_2, r_{12}) = \sum_{\ell=0}^{\infty} \left(n^\ell r_0^\ell\right)^\nu \times \left(1 + C_0 Zr_{12}\right) \exp[-\alpha(r_1 + r_2)]
\]

In this expression, \(n\) is the principal quantum number; \(\ell\) is orbital quantum number, \(r_0\) is Bohr radius, \(C_0\) and \(\alpha\) are the variational parameters to be determined by minimizing the energy, \(Z\) is the nuclear charge number, \(r_{12}\) represents the term electron-electron repulsion \(r_1\) and \(r_2\) are the coordinates of electrons with respect to the nucleus.
From the theoretical viewpoint, the Hylleraas variational method is based on the Hylleraas and Undheim theorem [31] according to which, a good approximation of the energy eigenvalue \( E(\alpha, C_0) \) is obtained when the minima of the function \( (d^2E(\alpha, C_0))/d\alpha dC_0 \) converge with increasing values of the dimension \( D \) of the basis states and when the function exhibit a plateau.

Using this theorem, the values of the variational parameters \( \alpha \) and \( C_0 \) can be determined by the following conditions:

\[
\frac{\partial E(\alpha, C_0)}{\partial C_0} = 0
\]

and

\[
\frac{\partial E(\alpha, C_0)}{\partial \alpha} = 0
\]

In the framework of the Ritz’ variation principle, the energy \( E(\alpha, C_0) = \langle \hat{H}(\alpha, C_0) \rangle \) is calculated from the relation:

\[
\langle \hat{H}(\alpha, C_0) \rangle = \left\langle \Psi(\alpha, C_0) \right| \hat{H} \left| \Psi(\alpha, C_0) \right\rangle
\]

In this equation, the correlated wave functions are given by (4) and the Hamiltonian \( \hat{H} \) of the helium isoelectronic series in given by (2) (in atomic units).

Furthermore, the closure relation represents the fact that \( |r_1, r_2 \rangle \) are continuous bases in the space of the two-electron space, written as follow:

\[
\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \Psi_1(r_1) \Psi_2(r_2) |r_1, r_2 \rangle \langle r_1, r_2| = 1
\]

Using this relation, according to (7), we obtain:

\[
E(\alpha, C_0) = \int \int dr_1^3 dr_2^3 \langle \Psi(\alpha, C_0) \rangle \hat{H} \langle \Psi(\alpha, C_0) \rangle
\]

By developing this expression (9), we find:

\[
E(\alpha, C_0) = \int \int dr_1^3 dr_2^3 \Psi(\alpha, C_0) \times \hat{H} \Psi(\alpha, C_0) = \int \int dr_1^3 dr_2^3 \Psi(\alpha, C_0) \hat{H} \Psi(\alpha, C_0)
\]

This means:

\[
N \ast E(\alpha, C_o) = \int \int dr_1^3 dr_2^3 \Psi(\alpha, C_0) \hat{H} \Psi(\alpha, C_0)
\]

with the normalization constant

\[
N = \int \int dr_1^3 dr_2^3 |\Psi(\alpha, C_0)|^2
\]

To make it easier to integrate Equation (11), we operate the variable changes in elliptic coordinates by:

\[
s = r_1 + r_2; \quad t = r_1 - r_2; \quad u = r_{12}
\]

On the basis of these variable changes, the elementary volume element

\[
d\tau = d^3r_1 d^3r_2 = 2\pi^2 \left( s^2 - t^2 \right) ududsdt
\]
Using these elliptical coordinates, Equation (11) is written as follows

\[
N\varepsilon (\alpha, C_0) = \int_0^\infty ds \int_0^\infty du \int_0^{s^2-t^2} \left[ u (s^2-t^2) \left( \frac{\partial^2 \Psi}{\partial s^2} + \frac{\partial^2 \Psi}{\partial t^2} + \frac{\partial^2 \Psi}{\partial u^2} \right) \right] ds \left( s^2 - u^2 \right) + t (s^2 - u^2) \left( \frac{\partial \Psi}{\partial s} + \frac{\partial \Psi}{\partial t} - \Psi \times \left( 4Zsu - s^2 + t^2 \right) \right)
\]

(15)

with respect to the correlated wave functions given by expression (4), it is expressed as follow

\[
\Psi(s,t,u,\alpha, C_0) = \sum_{i=0}^{\infty} \left( n_z^2 r_0^2 \right)^{u} (1 + C_0 Zu) \exp(-\alpha s)
\]

(16)

Furthermore, according to (12), the normalization constant is written in elliptic coordinates as:

\[
N = \int_0^\infty ds \int_0^\infty du \int_0^{s^2-t^2} \Psi^2 ds
\]

(17)

2.2. General Formalism of the SCUNC Method

The Screening Constant by Unit Nuclear Charge (SCUNC) formalism is used in this work to calculate the total energies of the symmetrical \((n\ell^2)\,^{1}\!L^\pi\) doubly excited states of the helium-isoelectronic up to \(Z = 10\).

In the framework of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism, total energies of the \((N\ell n\ell')\,^{2S+1}\!L^\pi\) doubly excited states are expressed in Rydberg (Ry) as below [24] [25]

\[
E(N\ell n\ell', \,^{2S+1}\!L^\pi) = -Z^2 \left( \frac{1}{N^2} + \frac{1}{n^2} \left[ 1 - \beta(N\ell n\ell', \,^{2S+1}\!L^\pi, Z) \right]^2 \right)
\]

(18)

In this equation, the principal quantum numbers \(N\) and \(n\), are respectively the inner and the outer electron of the helium-isoelectronic series. In this equation, the \(\beta\)-parameters are screening constant by unit nuclear charge expanded in inverse powers of \(Z\) and given by

\[
\beta(N\ell n\ell', \,^{2S+1}\!L^\pi, Z) = \sum_{k=1}^{4} f_k \left( \frac{1}{Z} \right)^k
\]

(19)

where \(f_k = f_k(N\ell n\ell', \,^{2S+1}\!L^\pi)\) are screening constants to be evaluated based on variational predicable using a wavefunction.

For the states \((n\ell^2)\,^{1}\!L^\pi\), \(N = n\) and \(l = l'\). Hence, the total energy is written as follow:

\[
E(n\ell^2, \,^{1}\!L^\pi) = -\frac{Z^2}{n^2} \left[ 1 + \left( 1 - \beta(n\ell^2, \,^{1}\!L^\pi, Z) \right)^2 \right] \text{Ry}
\]

(20)

Furthermore, in the framework of the screening constant by unit nuclear charge formalism, the \(\beta\)-screening constant is expressed in terms of the variational \(\alpha\)-parameter as follow

\[
\beta(n\ell^2, \,^{1}\!L^\pi, Z, \alpha) = \frac{\alpha}{Z^2} \left( 1 + \frac{2L}{2n+4L-3} \right)
\]

(21)
In this expression, \( n \) denotes the principal quantum number, \( L \) characterizes the considered quantum state (S, P, D, F etc.) and \( \alpha \) is the variational parameter.

Then, using Equation (21), the total energies of the symmetrical \((n\ell) \, ^1L^\pi\) doubly excited states in the helium isoelectronic series is expressed in Rydberg (Ry) as below:

\[
E(n\ell^2, ^1L^\pi, Z) = -\frac{Z^2}{n^2} \left[ 1 + \left( 1 - \frac{\alpha}{Z^2} \right) \left( 1 + \frac{2L}{2n+4L-3} \right)^2 \right] \text{Ry}
\]  

(22)

In this equation, only the parameter \( \alpha \) is unknown. Considering the \((2s^2) \, ^1S^\prime\) state of Helium-like ions \((Z = 2 \text{ - } 10)\), we calculated the values of the variational parameters \( \alpha \) and \( C_0 \), the results of which are presented in Table 1.

The Equation (22) is used to calculate the total energies of the \((n\ell^2) \, ^1L^\pi\) doubly excited states of helium-like ions without a complex calculation program.

3. Results and Discussions

The results obtained in the present study for \((ns^2) \, ^1S^\prime\), \((np^2) \, ^1D^\prime\), \((nf^2) \, ^1G^\prime\), \((nf^2) \, ^1I^\prime\), \((ng^2) \, ^1K^\prime\), and \((nh^2) \, ^1M^\prime\) with \( n \leq 20 \) in the helium-like ions up to \( Z = 10 \) are listed in Tables 1-16 and compared to various other calculations. Table 1 presents our results on the calculation of the variational parameters \( \alpha \) and \( C_0 \).

These variational parameters are calculated by determining the expression of \( E = f(\alpha, C_0) \) from the expression (15) and the wavefunction (16), then according to conditions (5) and (6) we obtained a system of equations whose resolution to give the values of the variational parameters \( \alpha \) and \( C_0 \) with \( 2 \leq Z \leq 10 \). All calculations in this work were performed with the calculation program MAXIMA. In Tables 2-7 we have listed our present results \( E \) on the calculation of the total energies of the \((n\ell^2) \, ^1L^\pi\) doubly excited states of the helium isoelectronic sequence with \( 2 \leq Z \leq 10 \) and \( 2 \leq n \leq 20 \) obtained using Equation (22). Table 2 shows our present results of the \((ns^2) \, ^1S^\prime\) \((n = 2 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\). Table 3 shows our present results of the \((np^2) \, ^1D^\prime\) \((n = 2 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\). Table 4 shows our present results of the \((nf^2) \, ^1G^\prime\) \((n = 3 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\). Table 5 shows our present results of the \((nf^2) \, ^1I^\prime\) \((n = 4 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\). Table 6 shows our present results of the \((ng^2) \, ^1K^\prime\) \((n = 5 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\). Table 7 shows our present results of the \((nh^2) \, ^1M^\prime\) \((n = 6 \text{ - } 20)\) doubly excited states of helium-like systems \((Z = 2 \text{ - } 10)\).

Table 8 shows a comparison of the present calculations for the \((ns^2) \, ^1S^\prime\) states with the results of the semi-empirical procedure of the screening constant by

| \( Z \) | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \( \alpha \) | 0.96105 | 1.40362 | 1.93837 | 2.47394 | 3.00997 | 3.54627 | 4.08276 | 4.61938 | 5.15608 |
| \( C_0 \) | 0.24982 | 0.26539 | 0.28139 | 0.29115 | 0.29771 | 0.30244 | 0.30600 | 0.30878 | 0.31102 |
Table 2. Total energy (−E) for (ns²) ¹S⁺ (n = 2 - 20) doubly excited states of helium-like systems (Z = 2 - 10). The energies E are in eV.

| Z | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   |
|---|------|------|------|------|------|------|------|------|------|
| ns² | −E   | −E   | −E   | −E   | −E   | −E   | −E   | −E   | −E   |
| 2⁺ | 21.45940 | 52.42726 | 96.46002 | 154.07753 | 225.28724 | 310.09472 | 408.50290 | 520.51348 | 646.12749 |
| 3⁺ | 9.53751 | 23.29900 | 42.87112 | 68.47890 | 100.12766 | 137.81987 | 181.55684 | 231.33932 | 287.16777 |
| 4⁺ | 5.36485 | 13.10569 | 24.11501 | 38.51938 | 56.32181 | 77.52368 | 102.12572 | 130.12837 | 161.53187 |
| 5⁺ | 3.43350 | 8.38764 | 15.43360 | 24.65241 | 36.04596 | 49.61515 | 65.36046 | 83.28216 | 103.38040 |
| 6⁺ | 2.38438 | 5.82475 | 10.71778 | 17.11973 | 25.03192 | 34.5497 | 45.38921 | 57.83483 | 71.79194 |
| 7⁺ | 1.75179 | 4.27941 | 7.87429 | 12.57767 | 18.39080 | 25.31385 | 33.34718 | 42.49090 | 52.74510 |
| 8⁺ | 1.34121 | 3.27642 | 6.02875 | 9.62985 | 14.08045 | 20.17298 | 25.70437 | 31.90753 | 40.38297 |
| 9⁺ | 1.05972 | 2.58878 | 4.73646 | 7.60877 | 11.12530 | 15.31332 | 20.17298 | 25.70437 | 31.90753 |
| 10⁺ | 0.85838 | 2.09691 | 3.85840 | 6.16310 | 9.01149 | 12.40379 | 16.34012 | 20.82054 | 25.84510 |

Table 3. Total energy (−E) for the (np²) ¹D⁺ (n = 2 - 20) doubly excited states of helium-like systems (Z = 2 - 10). The energies E are in eV.

| Z | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   |
|---|------|------|------|------|------|------|------|------|------|
| np² | −E   | −E   | −E   | −E   | −E   | −E   | −E   | −E   | −E   |
| 2⁺ | 19.40691 | 48.98779 | 91.46705 | 147.50214 | 217.11646 | 300.32082 | 397.12093 | 507.52007 | 631.52025 |
| 3⁺ | 8.78089 | 22.04020 | 41.04506 | 66.07698 | 97.14529 | 134.25433 | 177.40638 | 226.60274 | 281.84424 |
| 4⁺ | 5.00135 | 12.50334 | 23.24244 | 37.32758 | 54.89863 | 75.82286 | 100.14645 | 127.87008 | 158.99418 |
| 5⁺ | 3.23051 | 8.05224 | 14.94822 | 24.01485 | 35.25507 | 48.67024 | 64.26108 | 82.02799 | 101.97124 |
| 6⁺ | 2.25935 | 5.61862 | 10.41971 | 16.72838 | 24.54660 | 33.87526 | 44.71844 | 57.06561 | 70.92775 |
| 7⁺ | 1.66926 | 4.14359 | 7.67801 | 12.32015 | 18.07141 | 24.93241 | 32.90349 | 41.98486 | 52.17663 |
| 8⁺ | 1.28386 | 3.18216 | 5.89260 | 9.45120 | 13.85900 | 19.11648 | 25.22888 | 32.18135 | 39.98987 |
| 9⁺ | 1.01824 | 2.52067 | 4.66512 | 7.47977 | 10.96542 | 15.12242 | 19.95098 | 25.45121 | 31.62516 |
| 10⁺ | 0.82739 | 2.04609 | 3.78505 | 6.0690 | 8.89227 | 12.26146 | 16.17460 | 20.63180 | 25.63311 |
| 11⁺ | 0.68564 | 1.69405 | 3.13258 | 5.01981 | 7.35623 | 10.14210 | 13.37752 | 17.06258 | 21.19731 |
| 12⁺ | 0.57748 | 1.42570 | 2.63546 | 4.22227 | 6.18654 | 8.52846 | 11.24814 | 14.34564 | 17.82100 |
| 13⁺ | 0.49305 | 1.21645 | 2.24800 | 3.60082 | 5.27527 | 7.27152 | 9.58964 | 12.22970 | 15.19171 |
**Table 4.** Total energy ($-E$) for the \((nd^2) \, ^1\Sigma^+ \) \((n = 3 - 20)\) doubly excited states of helium-like systems \((Z = 2 - 10)\). The energies \(E\) are in eV.

| \(Z\) | \(2\) | \(3\) | \(4\) | \(5\) | \(6\) | \(7\) | \(8\) | \(9\) | \(10\) |
|---|---|---|---|---|---|---|---|---|---|
| \(3d^2\) | 8.66987 | 21.84944 | 40.76532 | 65.70667 | 96.68358 | 133.70073 | 176.76056 | 225.86449 | 281.01340 |
| \(4d^2\) | 4.92028 | 12.36512 | 23.04025 | 37.10354 | 54.56575 | 75.42399 | 99.68137 | 127.33865 | 158.39628 |
| \(5d^2\) | 3.17227 | 7.95352 | 14.80410 | 23.82457 | 35.01823 | 48.38660 | 63.93048 | 81.65034 | 101.54646 |
| \(6d^2\) | 2.16707 | 5.46666 | 10.31481 | 16.59001 | 24.37447 | 33.66919 | 44.47473 | 56.79139 | 70.61936 |
| \(7d^2\) | 1.63727 | 4.08980 | 7.59970 | 12.21693 | 17.94306 | 24.77881 | 32.72457 | 41.78056 | 51.94691 |
| \(8d^2\) | 1.25931 | 3.14100 | 5.83274 | 9.37235 | 13.76099 | 18.99922 | 25.08731 | 32.02543 | 39.81368 |
| \(9d^2\) | 0.99901 | 2.48852 | 4.61839 | 7.41825 | 10.88897 | 15.03099 | 19.84451 | 25.32967 | 31.48654 |
| \(10d^2\) | 0.81206 | 2.02051 | 3.74790 | 6.01801 | 8.83154 | 12.18833 | 16.09005 | 20.53529 | 25.52462 |
| \(11d^2\) | 0.67323 | 1.67337 | 3.10257 | 4.98032 | 7.30720 | 10.08347 | 13.30928 | 16.98469 | 21.0977 |
| \(12d^2\) | 0.56728 | 1.40875 | 2.61088 | 4.18993 | 6.46393 | 8.48047 | 11.19228 | 14.28189 | 17.74935 |
| \(13d^2\) | 0.48458 | 1.20239 | 2.22761 | 3.57401 | 5.24199 | 7.23174 | 9.54334 | 12.17686 | 15.13234 |
| \(14d^2\) | 0.41878 | 1.03834 | 1.92304 | 3.08470 | 4.52364 | 6.24003 | 8.23394 | 10.50542 | 13.05450 |
| \(15d^2\) | 0.36555 | 0.90576 | 1.67701 | 2.68951 | 3.94357 | 5.43931 | 7.17681 | 9.15611 | 11.37723 |
| \(16d^2\) | 0.32189 | 0.79709 | 1.47539 | 2.63575 | 3.46841 | 4.78350 | 6.31106 | 8.05115 | 10.00378 |
| \(17d^2\) | 0.28563 | 0.70689 | 1.30810 | 2.09717 | 3.07430 | 4.23960 | 5.93311 | 7.13489 | 8.86493 |
| \(18d^2\) | 0.25518 | 0.63119 | 1.16777 | 1.87190 | 2.74378 | 3.78351 | 4.99112 | 6.36666 | 7.91012 |
| \(19d^2\) | 0.22936 | 0.56706 | 1.04888 | 1.68110 | 2.46388 | 3.39729 | 4.48139 | 5.71620 | 7.10173 |
| \(20d^2\) | 0.20728 | 0.51223 | 0.94729 | 1.51807 | 2.22474 | 3.06737 | 4.04598 | 5.16061 | 6.41126 |

**Table 5.** Total energy \((−E)\) for the \((nf^2) \, ^1\Pi \) \((n = 4 - 20)\) doubly excited states of helium-like systems \((Z = 2 - 10)\). The energies \(E\) are in eV.

| \(Z\) | \(2\) | \(3\) | \(4\) | \(5\) | \(6\) | \(7\) | \(8\) | \(9\) | \(10\) |
|---|---|---|---|---|---|---|---|---|---|
| \(4f^2\) | 4.88462 | 12.30381 | 22.95032 | 36.98626 | 54.41728 | 75.24595 | 99.47366 | 127.10120 | 158.12904 |
| \(5f^2\) | 3.14469 | 7.90632 | 14.73497 | 23.73314 | 34.90428 | 48.25001 | 63.77119 | 81.46828 | 101.31460 |
| \(6f^2\) | 2.19522 | 5.51005 | 10.26127 | 16.51924 | 24.28632 | 33.56358 | 44.35159 | 56.65069 | 70.46106 |
| \(7f^2\) | 1.62030 | 4.06908 | 7.55759 | 12.16131 | 17.87382 | 24.69587 | 32.62789 | 41.67010 | 51.82266 |
| \(8f^2\) | 1.24569 | 3.11795 | 5.79909 | 9.32793 | 13.70571 | 18.93303 | 25.01016 | 31.93731 | 39.71456 |
Continued

Table 6. Total energy \((-E)\) for the \((ng^2)\) \(1K^\prime\) \((n = 5 - 20)\) doubly excited states of helium-like systems \((Z = 2 - 10)\). The energies \(E\) are in eV.

| \(Z\) | \(2\) | \(3\) | \(4\) | \(5\) | \(6\) | \(7\) | \(8\) | \(9\) | \(10\) |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(ng^2\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) |
| 5g\(^2\) | 3.12860 | 7.87865 | 14.69439 | 23.67940 | 34.83728 | 48.16967 | 63.67745 | 81.36112 | 101.22099 |
| 6g\(^2\) | 2.18229 | 5.48788 | 10.22878 | 16.47627 | 24.23275 | 33.49937 | 44.27669 | 56.56508 | 70.36472 |
| 7g\(^2\) | 1.60979 | 4.04301 | 7.53129 | 12.12654 | 17.83049 | 24.63495 | 32.56734 | 41.60091 | 51.74480 |
| 8g\(^2\) | 1.23704 | 3.10320 | 5.77753 | 9.29943 | 13.67022 | 18.89050 | 24.96058 | 31.88065 | 39.65082 |
| 9g\(^2\) | 0.98071 | 2.45755 | 4.57320 | 7.35860 | 10.8474 | 14.9249 | 19.74091 | 25.21133 | 31.35343 |
| 10g\(^2\) | 0.79685 | 1.99482 | 3.71044 | 5.96858 | 8.77005 | 12.11521 | 16.00426 | 20.43731 | 25.41443 |
| 11g\(^2\) | 0.66044 | 1.65182 | 3.07117 | 4.93891 | 7.25569 | 10.02181 | 13.23743 | 16.90264 | 21.0750 |
| 12g\(^2\) | 0.55643 | 1.39049 | 2.58428 | 4.15487 | 6.10279 | 8.42829 | 11.13149 | 14.21248 | 17.67130 |
| 13g\(^2\) | 0.47529 | 1.18677 | 2.04888 | 3.54406 | 5.20475 | 7.18718 | 9.49144 | 12.11760 | 15.06570 |
| 14g\(^2\) | 0.41075 | 1.02488 | 1.90347 | 3.05891 | 4.49158 | 6.20167 | 8.18926 | 10.45441 | 12.99715 |
| 15g\(^2\) | 0.35858 | 0.89408 | 1.66002 | 2.66713 | 3.91576 | 5.40604 | 7.13807 | 9.11888 | 11.32750 |
| 16g\(^2\) | 0.31579 | 0.78687 | 1.46055 | 2.34621 | 3.44413 | 4.75445 | 6.27724 | 8.01254 | 9.96037 |
| 17g\(^2\) | 0.28026 | 0.69791 | 1.29506 | 2.08000 | 3.05297 | 4.21408 | 5.56341 | 7.10097 | 8.82681 |
| 18g\(^2\) | 0.25042 | 0.62326 | 1.15624 | 1.85673 | 2.72494 | 3.76097 | 4.96489 | 6.33671 | 7.87646 |
| 19g\(^2\) | 0.22513 | 0.56001 | 1.03865 | 1.66763 | 2.44715 | 3.37297 | 4.5810 | 5.68962 | 7.07185 |
| 20g\(^2\) | 0.20350 | 0.50594 | 0.93816 | 1.50606 | 2.20982 | 3.04952 | 4.02521 | 5.13690 | 6.38462 |

Table 7. Total energy \((-E)\) for the \((nh^2)\) \(1M^\prime\) \((n = 6 - 20)\) doubly excited states of helium-like systems \((Z = 2 - 10)\). The energies \(E\) are in eV.

| \(Z\) | \(2\) | \(3\) | \(4\) | \(5\) | \(6\) | \(7\) | \(8\) | \(9\) | \(10\) |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(ng^2\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) | \(-E\) |
| 6h\(^2\) | 2.17365 | 5.47302 | 10.20698 | 16.44740 | 24.19675 | 33.45620 | 44.22633 | 56.50750 | 70.29992 |
| 7h\(^2\) | 1.60263 | 4.03075 | 7.51331 | 12.10275 | 17.80083 | 24.60839 | 32.52856 | 41.55350 | 51.69145 |
Table 8. Comparison of the present calculations on total energies of the doubly (ns²) ¹S¹ systems (Z = 2 - 10) with available literature values. All results are expressed in eV.

| States | ns² ¹S¹ | Z   | 2     | 3     | 4     | 5     | 6     | 7     | 8     | 9     | 10     |
|--------|---------|-----|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| −𝑃     | 21.45940| 52.42276 | 96.46002 | 154.07753 | 225.28724 | 310.09472 | 408.50290 | 520.51348 | 646.12749 |
| −𝑃     | 21.19004 | 51.75672 | 95.92923 | 153.70728 | 225.09117 | 310.08075 | 408.67588 | 520.87683 | 646.68334 |
| −𝑃     | 21.16692 | 51.86067 | 96.15032 | 154.04035 | 225.53336 | 310.63042 | 409.33154 | 521.63766 | 647.54894 |
| −𝑃     | 21.19388 | 51.75719 | 95.92188 | 153.72003 | 225.09205 | 310.08931 | 408.67561 | 520.87758 | 646.68514 |
| −𝑃     | 21.16678 | 51.86054 | 96.15046 | 154.03995 | 225.53363 | 310.62879 | 409.33289 | 521.62923 | 647.54853 |
| −𝑃     | 21.16460 | 51.86312 | 96.14556 | 154.03886 | 225.53540 | 310.62852 | 409.33358 | 521.63576 | 647.54377 |
| −𝑃     | 21.19000 | 52.00000 | 96.43000 | 154.45000 | 226.09000 | 311.32000 | 410.17000 | 522.62000 | 648.67000 |
| −𝑃     | 9.35725  | 23.29900 | 42.87112 | 68.47890 | 100.12766 | 137.81987 | 181.55684 | 231.33932 | 287.16777 |
| −𝑃     | 9.64652  | 23.38097 | 43.16324 | 68.99254 | 100.86877 | 138.79205 | 182.76224 | 232.77934 | 288.84349 |
| −𝑃     | 9.64065  | 23.48066 | 43.29425 | 69.06061 | 100.76559 | 138.39575 | 181.93676 | 231.37273 | 286.68564 |
| −𝑃     | 9.62031  | 23.40586 | 43.23344 | 69.10874 | 101.02769 | 138.99573 | 183.00878 | 233.07901 | 289.17806 |
| −𝑃     | 9.41772  | 23.03000 | 42.63519 | 68.31431 | 100.04059 | 137.81366 | 181.63365 | 231.50082 | 287.41489 |
| −𝑃     | 9.62017  | 23.40586 | 43.23316 | 69.10847 | 101.02837 | 138.99627 | 183.00918 | 233.06996 | 289.17887 |
| −𝑃     | 9.62466  | 23.40178 | 43.22527 | 69.10738 | 101.02224 | 138.98212 | 182.99653 | 233.05866 | 289.17125 |
| −𝑃     | 9.58385  | 22.83852 | 42.25657 | 67.85978 |         |         |         |         |         |
| −𝑃     | 9.42000  | 23.11000 | 42.86000 | 68.65000 | 100.48000 | 138.37000 | 182.30000 | 232.27000 | 288.30000 |
| −𝑃     | 5.36485  | 13.10569 | 24.11501 | 38.51938 | 56.32181 | 77.52368 | 102.12572 | 130.12837 | 161.53187 |
| −𝑃     | 5.49139  | 13.25971 | 24.42944 | 39.00059 | 56.97332 | 78.34732 | 103.12276 | 131.29961 | 162.87803 |
| −𝑃     | 5.46963  | 13.25848 | 24.45079 | 39.03978 | 57.02243 | 78.41957 | 103.20357 | 131.40206 | 162.99422 |
| −𝑃     | 5.29751  | 12.93915 | 23.98235 | 38.42684 | 56.27276 | 77.52023 | 102.16899 | 131.21932 | 161.67093 |
Continued

| \( n^2 \, 1S^0 \) | \( n^2 \, 1S^0 \) | \( n^2 \, 1S^0 \) | \( n^2 \, 1S^0 \) |
|---|---|---|---|
| \( -E \) | 5.5000 | 13.18000 | 24.49000 | 38.08000 | 57.95000 | 78.43000 | 103.18000 | 130.42000 | 163.20000 |
| \( -P^0 \) | 5.30000 | 13.00000 | 24.11000 | 38.61000 | 56.52000 | 77.83000 | 102.54000 | 130.65000 | 162.17000 |
| \( -E^0 \) | 3.43350 | 8.38764 | 15.43360 | 24.65241 | 36.04596 | 49.61515 | 65.36046 | 83.28216 | 103.38040 |
| \( 5^2 \, 1S^0 \) | \( -P^0 \) | 3.53993 | 8.28111 | 15.34872 | 24.59325 | 36.01455 | 49.61291 | 65.38816 | 83.34034 | 103.46942 |
| \( 6^2 \, 1S^0 \) | \( -P^0 \) | 3.39000 | 8.32000 | 15.43000 | 24.71000 | 36.17000 | 49.81000 | 65.63000 | 83.62000 | 103.79000 |
| \( 7^2 \, 1S^0 \) | \( -P^0 \) | 2.38438 | 5.82475 | 10.71778 | 17.11973 | 25.03192 | 34.45497 | 45.38921 | 57.83483 | 71.79194 |
| \( P^0 \) | 2.47025 | 5.94161 | 10.92483 | 17.41965 | 25.42606 | 34.94460 | 45.97447 | 58.51647 | 72.57007 |
| \( E^0 \) | 2.35000 | 5.78000 | 10.71000 | 17.16000 | 25.12000 | 34.59000 | 45.57000 | 58.07000 | 72.07000 |
| \( 6^2 \, 1S^0 \) | \( -P^0 \) | 1.72000 | 4.27000 | 7.82000 | 12.63000 | 18.46000 | 25.41000 | 33.48000 | 42.66000 | 52.95000 |
| \( P^0 \) | 1.73000 | 4.24000 | 7.87000 | 12.61000 | 18.46000 | 25.41000 | 33.48000 | 42.66000 | 52.95000 |
| \( E^0 \) | 1.821259 | 4.37559 | 8.04042 | 12.81602 | 18.70239 | 25.69953 | 33.80717 | 43.02557 | 53.35447 |

\(^{1}\text{Present work, values calculated from Equation (22)}, ^{2}\text{Sakho [32]}, ^{3}\text{Ho [33]}, ^{4}\text{Sow et al. [36]}, ^{5}\text{Gning et al. [37]}, ^{6}\text{Konté et al. [38]}, ^{7}\text{Ho [34]}, ^{8}\text{Sakho et al. [24]}, ^{9}\text{Ray et al. [23]}, ^{10}\text{Ho [35]}, ^{11}\text{Diouf et al. [39]}, ^{12}\text{Sakho [40]}.\)

\(^{1}\text{Present work, values calculated from Equation (22)}, ^{2}\text{Sakho [32]}, ^{3}\text{Ho [33]}, ^{4}\text{Sow et al. [36]}, ^{5}\text{Gning et al. [37]}, ^{6}\text{Konté et al. [38]}, ^{7}\text{Ho [34]}, ^{8}\text{Sakho et al. [24]}, ^{9}\text{Ray et al. [23]}, ^{10}\text{Ho [35]}, ^{11}\text{Diouf et al. [39]}, ^{12}\text{Sakho [40]}.\)

In Table 9, we compare our calculations for \((np^2) \, 1D^0\) states with the results of the complex rotation of Ho [33] [34] [35], with the results of Sow et al. [36] who used the variational method of the SCUNC formalism, with the complex rotation values of Gning et al. [37], with the Konté et al. [38] data, with the data from the time-dependent variation perturbation theory of Ray et al. [23], with the results of Diouf et al. [39] and finally with the data from the modified slater theory of Sakho [40]. The observation of our results shown in this table shows that our present calculations are generally in good agreement with the results of the cited authors up to \(Z = 10\).

In Table 9, we compare our calculations for \((np^2) \, 1D^0\) states with the results of the calculations of Badiane et al. [41], with the data of Sakho [24] [32] [40], with the results of the complex rotation calculations (CRC) of Ho and Bhatia [13], with the values of Ivanov and Safronova [17], with the results of the variational method calculations of Hylleraas de Biaye et al. [16] and finally with those obtained by Roy et al. [18] who applied the functional density theory (FDT). Here, the agreements between the calculations are considered good. Table 10 compares our results for the \((n^2d) \, 1G^+ (n = 3 - 10)\) states with those obtained by Badiane et al. [41], Sakho [32] [40], Bachau et al. [19], Biaye et al. [16], Ivanov and Safronova [17], Diouf et al. [39], Ray et al. [23] and Roy et al. [18]. As regards the \((n^2d) \, 1G^+\) levels, comparison shows also a good agreement up to \(Z = 10\). Table 11 shows the results of our present calculations of the total energies of the doubly excited \((n^2f) \, 1I^+ (n = 4 - 10)\) states of helium-like systems up to \(Z = 10\), which we compare with those obtained by Biaye et al. [16], Badiane et al. [41], Sakho et al. [32] [40], Ho [20], Diouf et al. [39], and Sow et al. [36]. A comparative
Table 9. Comparison of the present calculations on total energies of the doubly \((np^2)^1\text{D}_r\) \((n = 2 - 5)\) excited states of helium-like systems \((Z = 2 - 10)\) with available literature values. All results are expressed in eV.

| States \(np^2 1\text{D}_r\) | \(Z\) | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----------------------------|-----|---|---|---|---|---|---|---|---|----|
| \(-E^p\)                    | 19.40971 | 48.98779 | 91.46705 | 147.50214 | 217.11646 | 300.32082 | 397.12093 | 507.52007 | 631.52025 |
| \(-E^p\)                    | 19.12145 | 48.19274 | 90.86974 | 147.15243 | 217.04218 | 300.53626 | 397.63604 | 508.34153 | 632.65271 |
| \(-E^p\)                    | 19.12008 | 48.19002 | 90.86656 | 147.14835 | 217.03537 | 300.52809 | 397.62652 | 508.33201 | 632.64183 |
| \(-E^p\)                    | 19.10104 | 48.18049 | 90.81665 | 147.13835 | 217.02869 | 300.26551 | 397.28229 | 507.90071 | 632.12481 |
| \(-E^p\)                    | 19.14533 | 48.39138 | 90.97314 | 147.16059 | 216.95238 | 300.35123 | 397.35577 | 507.96601 | 632.18195 |
| \(-E^p\)                    | 19.18403 | 48.39138 | 91.14321 | 147.47352 | 217.39320 | 300.90769 | 398.02245 | 508.73746 | 633.05408 |
| \(-E^p\)                    | 47.78049 | 90.54592 | 146.90888 |                  |                  |                  |                  |                  |                  |
| \(-E^p\)                    | 19.12000 | 48.19000 | 90.87000 | 147.15000 | 217.03000 | 300.53000 | 397.63000 | 508.33000 | 632.64000 |
| \(-E^p\)                    | 19.12000 | 48.73000 | 91.95000 | 147.87000 | 219.20000 | 303.24000 | 400.88000 | 512.13000 | 636.98000 |
| \(-E^p\)                    | 8.78089  | 22.04020 | 41.04506 | 66.07698  | 97.14529  | 134.25433 | 177.40638 | 226.60274 | 281.84424 |
| \(-E^p\)                    | 8.98656  | 22.56777 | 42.23345 | 67.96182  | 99.74201  | 137.57401 | 181.45511 | 231.38394 | 287.36187 |
| \(-E^p\)                    | 9.33759  | 27.62192 | 42.10011 | 67.62440  | 99.19642  | 136.81482 | 180.48094 | 230.19344 | 285.95368 |
| \(-E^p\)                    | 8.66955  | 21.82626 | 40.49669 | 66.40669  | 97.38993  | 134.42000 | 179.18160 | 229.06009 | 285.07883 |
| \(-E^p\)                    | 8.50000  | 21.42000 | 40.38000 | 65.40000  | 96.46000  | 133.57000 | 176.72000 | 225.92000 | 281.17000 |
| \(-E^p\)                    | 5.00135  | 12.50334 | 23.24244 | 37.32587  | 54.89863  | 75.82286  | 100.14654 | 127.87008 | 158.99418 |
| \(-E^p\)                    | 12.8881  | 23.97187 | 38.52433 | 56.48269  | 77.84364  | 102.61009 | 130.77661 | 162.34727 |
| \(-E^p\)                    | 3.23051  | 8.05224  | 14.94822 | 24.01485  | 35.25507  | 48.67024  | 64.26108  | 82.02799  | 101.97124 |
| \(-E^p\)                    | 3.28849  | 8.24777  | 15.40029 | 24.73652  | 36.25238  | 49.94652  | 65.81892  | 83.86824  | 104.09583 |
| \(-E^p\)                    | 3.53068  | 8.51309  | 15.67240 | 25.00863  | 36.52178  | 50.21047  | 66.07743  | 84.12131  | 104.34209 |
| \(-E^p\)                    | 7.95117  | 14.92953 | 24.08344 |                  |                  |                  |                  |                  |                  |
| \(-E^p\)                    | 7.71000  | 14.54000 | 23.54000 | 34.72000  | 48.08000  | 63.62000  | 81.33000  | 101.22000 |
| \(-E^p\)                    | 3.06000  | 7.80000  | 14.71000 | 23.80000  | 35.07000  | 48.52000  | 64.14000  | 81.94000  | 101.92000 |

1Present work, values calculated from Equation (22), aBadiane et al. [41], bSakho et al. [32], cHo and Bhatia [13], dIvanov and Safronova [17], eBiaye et al. [16], fRoy et al. [18], gSakho et al. [24], hSakho [40].
Table 10. Comparison of the present calculations on total energies of the doubly \((nd^2)^1\text{Ge}\) \((n = 3 - 10)\) excited states of helium-like systems \((Z = 2 - 10)\) with available literature values. All results are expressed in eV.

| States \(nd^2^1\text{Ge}\) | \(Z\) | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------------------------|-----|---|---|---|---|---|---|---|---|----|
| \(-F\) 3\(d^2\)^1\text{Ge} | 8.66987 | 21.84944 | 40.76532 | 65.70667 | 96.68358 | 133.70073 | 176.76056 | 225.86449 | 281.01340 | 321.32901 |
| \(-F\) 4\(d^2\)^1\text{Ge} | 8.31716 | 20.87794 | 39.56401 | 64.34271 | 95.23988 | 132.11133 | 175.08356 | 224.11306 | 279.19300 | 319.21848 |
| \(-F\) 5\(d^2\)^1\text{Ge} | 8.30942 | 21.07114 | 39.88374 | 64.74271 | 95.64942 | 132.60385 | 175.64667 | 225.61854 | 280.70732 | 320.73279 |
| \(-E\) 3\(d^2\)^1\text{Ge} | 8.38927 | 21.14053 | 39.89191 | 64.74814 | 95.48479 | 132.35685 | 175.32166 | 224.76232 | 279.28772 | 319.31317 |
| \(-E\) 4\(d^2\)^1\text{Ge} | 8.38383 | 21.54734 | 40.49464 | 65.45157 | 96.43174 | 133.44332 | 176.49175 | 225.57839 | 280.70732 | 320.73279 |
| \(-E\) 5\(d^2\)^1\text{Ge} | 8.57703 | 21.24938 | 39.97082 | 64.73727 | 95.51456 | 132.41065 | 175.26860 | 224.27632 | 279.28772 | 320.73279 |

\(^{1}\)Present work, values calculated from Equation (22), \(^{2}\)Badiane et al. [41], \(^{3}\)Sakho et al. [32], \(^{4}\)Bachau et al. [19], \(^{5}\)Biaye et al. [16], \(^{6}\)Ivanov and Safronova [17], \(^{7}\)Diouf et al. [39], \(^{8}\)Ray et al. [23], \(^{9}\)Roy et al. [18], \(^{10}\)Sakho [40].
### Table 11. Comparison of the present calculations on total energies of the doubly $^{1}I_e (n = 4 - 10)$ excited states of helium-like systems ($Z = 2 - 10$) with available literature values. All results are expressed in eV.

| States $nf^{2} \ ^{1}I_{e}$ | $Z$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----------------------------|----|---|---|---|---|---|---|---|---|----|
| $4f^{2} \ ^{1}I_{e}$       | $^{a}$ | 4.88462 | 12.30381 | 22.95032 | 36.98626 | 54.41728 | 75.24595 | 99.47366 | 127.10120 | 158.12904 |
| $5f^{2} \ ^{1}I_{e}$       | $^{a}$ | 5.02139 | 12.43411 | 22.78972 | 37.66355 | 55.38959 | 75.43250 | 100.78073 | 128.41943 | 159.33212 |
| $6f^{2} \ ^{1}I_{e}$       | $^{a}$ | 5.20000 | 12.56000 | 23.01000 | 37.86000 | 55.50000 | 75.68000 | 101.17735 | 128.70000 | 159.63000 |
| $7f^{2} \ ^{1}I_{e}$       | $^{a}$ | 5.30000 | 12.69000 | 23.22000 | 38.06000 | 55.70000 | 75.93000 | 101.73000 | 129.20000 | 160.03000 |
| $8f^{2} \ ^{1}I_{e}$       | $^{a}$ | 5.40000 | 12.82000 | 23.42000 | 38.26000 | 55.90000 | 76.18000 | 102.28000 | 129.70000 | 160.33000 |
| $9f^{2} \ ^{1}I_{e}$       | $^{a}$ | 5.50000 | 12.95000 | 23.62000 | 38.46000 | 56.10000 | 76.43000 | 102.83000 | 130.20000 | 160.63000 |
| $10f^{2} \ ^{1}I_{e}$      | $^{a}$ | 0.80291 | 2.00511 | 3.72546 | 5.98842 | 8.79474 | 12.14478 | 16.03872 | 20.47668 | 25.45872 |

$^{a}$Present work, values calculated from Equation (22), $^{b}$Biaye et al. [16], $^{c}$Radiane et al. [41], $^{d}$Sakho et al. [32], $^{e}$Ho [20], $^{f}$Diouf et al. [39], $^{g}$Sow et al. [36]; $^{h}$Sakho [40].

A reading of the results mentioned in this table shows a good agreement between the present SCUNC results and the data found in the literature. For level $4f^{2}$, it should be noted that comparison with the results of Biaye et al. [16] indicates satisfactory agreement for $Z = 2 - 10$.

In Table 12 and Table 13, we compare the results of our calculations of the total energies of the doubly excited states ($ng^{2}$) $^{1}K_{e}$ and ($n\ell^{2}$) $^{1}M_{e}$ with those of Sakho [40] and Diouf et al. [39]. The agreements between the calculations are seen to be generally good. It is worth mentioning that there are not many results.
### Table 12
Comparison of the present calculations on total energies of the doubly \((ng^2)^1K^+\) \((n = 5 - 10)\) excited states of helium-like systems \((Z = 2 - 10)\) with available literature values. All results are expressed in eV.

| States \((ng^2)^1K^+\) | \(Z\) | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------------|------|---|---|---|---|---|---|---|---|----|
| \(5g^2 1K^+\)         | \(E_p\) | 3.12860 | 7.87865 | 14.69439 | 23.67940 | 34.83728 | 48.16967 | 63.67745 | 81.36112 | 101.22099 |
|                        | \(E_a\) | 2.93000 | 7.59000 | 14.40000 | 23.40000 | 34.60000 | 47.90000 | 63.70000 | 81.24000 | 101.28000 |
|                        | \(E_b\) | 2.93000 | 7.59000 | 14.41000 | 23.41000 | 34.69000 | 47.90000 | 63.71000 | 81.24000 | 101.28000 |
| \(6g^2 1K^+\)         | \(E_p\) | 2.18229 | 5.48788 | 10.22878 | 16.47627 | 24.23275 | 33.49937 | 44.27669 | 56.56508 | 70.36472 |
|                        | \(E_a\) | 2.03000 | 5.27000 | 10.02000 | 16.27000 | 24.05000 | 33.30000 | 44.12000 | 56.43000 | 70.25000 |
|                        | \(E_b\) | 2.04000 | 5.23000 | 10.04000 | 16.22000 | 24.10000 | 33.41000 | 44.22000 | 56.54000 | 70.38000 |
| \(7g^2 1K^+\)         | \(E_p\) | 1.60979 | 4.04301 | 7.53129 | 12.12654 | 17.83049 | 24.64395 | 32.56734 | 41.60091 | 51.74480 |
|                        | \(E_a\) | 1.49000 | 3.87000 | 7.36000 | 11.96000 | 17.67000 | 24.49000 | 32.42000 | 41.46000 | 51.61000 |
|                        | \(E_b\) | 1.50000 | 3.88000 | 7.36000 | 11.95000 | 17.75000 | 24.43000 | 32.48000 | 41.51000 | 51.63000 |
| \(8g^2 1K^+\)         | \(E_p\) | 1.23704 | 3.10320 | 5.77753 | 9.29943 | 13.67022 | 18.89050 | 24.96058 | 31.88065 | 39.65082 |
|                        | \(E_a\) | 1.08071 | 2.45755 | 4.57320 | 7.35860 | 10.81474 | 14.94209 | 19.74091 | 25.21133 | 31.35343 |
|                        | \(E_b\) | 0.98685 | 1.99482 | 3.71044 | 5.96858 | 8.77005 | 12.11521 | 16.00426 | 20.43731 | 25.41443 |

1Present work, values calculated from Equation (22), aSakho [40], bDiouf et al. [39].

### Table 13
Comparison of the present calculations on total energies of the doubly \((nh^2)^1M^+\) \((n = 6 - 10)\) excited states of helium-like systems \((Z = 2 - 10)\) with available literature values. All results are expressed in eV.

| States \((nh^2)^1M^+\) | \(Z\) | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------------|------|---|---|---|---|---|---|---|---|----|
| \(6h^2 1M^+\)         | \(E_p\) | 2.17365 | 5.47302 | 10.20698 | 16.44740 | 24.19675 | 33.45620 | 44.22633 | 56.50750 | 70.29992 |
|                        | \(E_a\) | 2.02000 | 5.25000 | 9.99000 | 16.24000 | 24.01000 | 33.28000 | 44.07000 | 56.37000 | 70.18000 |
|                        | \(E_b\) | 2.04000 | 5.23000 | 9.97000 | 16.22000 | 24.10000 | 33.27000 | 44.06000 | 56.37000 | 70.18000 |
| \(7h^2 1M^+\)         | \(E_p\) | 1.60263 | 4.03075 | 7.51331 | 12.10275 | 17.80083 | 24.60839 | 32.52586 | 41.53550 | 51.69145 |
|                        | \(E_a\) | 1.48000 | 3.86000 | 7.34000 | 11.93000 | 17.64000 | 24.45000 | 32.38000 | 41.42000 | 51.56000 |
|                        | \(E_b\) | 1.46000 | 3.82000 | 7.36000 | 11.95000 | 17.63000 | 24.43000 | 32.33000 | 41.51000 | 51.63000 |
| \(8h^2 1M^+\)         | \(E_p\) | 1.23105 | 3.09296 | 5.76253 | 9.27960 | 13.64551 | 18.86088 | 24.92603 | 31.84117 | 39.60369 |
|                        | \(E_a\) | 0.97565 | 2.44891 | 4.56056 | 7.34189 | 10.79392 | 14.91715 | 19.71182 | 25.17808 | 31.31603 |
|                        | \(E_b\) | 0.79253 | 1.98746 | 3.69968 | 5.95436 | 8.75234 | 12.09399 | 15.97952 | 20.49094 | 25.38263 |

1Present work, values calculated from Equation (22), aSakho [40], bDiouf et al. [39].

on the states and the only ones available to our knowledge are those of the authors Sakho [40] and Diouf et al. [39]. Moreover for \(n > 7\) there are no results available so we think that the results cited up to \(n = 20\) in this work may be interesting for future experimental and theoretical studies on these states.

In Tables 14-16 are quoted results for excitation energies of helium-like ions with \(Z \leq 10\). Our excitation energies are calculated with respect to the accurate ground state energies of Frankowski and Pekeris [42]. Comparison indicates that our excitation energies for \((ns^2)^1S^+\), \((np^2)^1D^+\) and \((nd\ell)^1G^2\) levels agree well
Table 14. Comparison of the present calculations on the variational calculation of the excitation energies of the doubly excited states \((ns^2)^1S^0\) \((n = 2 - 5)\) of the He-like systems with some theoretical results available in the literature consulted for \(Z = 2 - 5\). All the results are expressed in eV: 1 Ryd = 13.605698 eV.

| States \(ns^2)^1S^0\) | \(Z\) | 2 | 3 | 4 | 5 |
|------------------------|------|---|---|---|---|
| \(2s^2)^1S^0\)         | \(E^f\) | 57.5548 | 145.6737 | 275.1269 | 445.4159 |
|                        | \(E^p\) | 57.8487 | 146.2476 | 275.4882 | 445.5893 |
|                        | \(E^d\) | 58.6460 | 147.7633 | 277.6814 | 448.4165 |
|                        | \(E^b\) | 57.8200 | 146.3400 | 275.6600 | 445.7800 |
| \(3s^2)^1S^0\)         | \(E^f\) | 69.4768 | 174.7975 | 328.7157 | 531.0145 |
|                        | \(E^p\) | 69.4299 | 175.2577 | 329.3314 | 531.6345 |
|                        | \(E^d\) | 69.9000 | 175.1000 | 328.9600 | 531.1800 |
|                        | \(E^b\) | 69.3972 | 174.7026 | 328.4035 | 530.5215 |
| \(4s^2)^1S^0\)         | \(E^f\) | 73.5469 | 184.8470 | 347.1820 | 560.5819 |
|                        | \(E^p\) | 73.4218 | 184.9939 | 347.5358 | 561.0999 |
|                        | \(E^d\) | 73.7100 | 185.1600 | 347.6100 | 561.0600 |
|                        | \(E^e\) | 75.5808 | 189.7089 | 356.1533 | 574.8140 |
| \(5s^2)^1S^0\)         | \(E^f\) | 75.1905 | 189.4457 | 355.9523 | 574.7972 |
|                        | \(E^p\) | 75.6200 | 189.8200 | 356.2400 | 574.9000 |

\(^a\)Present work, \(^b\)Ho [33], \(^c\)Ray and Mukherjee [23], \(^d\)Sakho et al. [24], \(^e\)Ho [34].

Table 15. Comparison of the present calculations on the variational calculation of the excitation energies of the doubly excited states \((np^2)^1D^0\) \((n = 2 - 5)\) of the He-like systems with some theoretical results available in the literature consulted for \(Z = 2 - 5\). All the results are expressed in eV: 1 Ryd = 13.605698 eV.

| States \(np^2)^1D^0\) | \(Z\) | 2 | 3 | 4 | 5 |
|------------------------|------|---|---|---|---|
| \(2p^2)^1D^0\)         | \(E^f\) | 59.6074 | 149.1087 | 280.1198 | 451.9913 |
|                        | \(E^p\) | 59.8900 | 149.9100 | 280.7200 | 452.3400 |
|                        | \(E^d\) | 149.9157 | 280.7699 | 452.4575 |
|                        | \(E^b\) | 60.3249 | 150.6749 | 281.6815 | 453.8316 |
|                        | \(E^e\) | 150.3239 | 281.0420 | 452.5854 |
|                        | \(E^f\) | 150.0599 | 280.9522 | 452.6670 |
| \(3p^2)^1D^0\)         | \(E^f\) | 70.2334 | 176.0563 | 330.5418 | 533.4165 |
|                        | \(E^p\) | 70.5100 | 176.6900 | 331.2100 | 534.0900 |
|                        | \(E^d\) | 176.4251 | 330.8008 | 533.5502 |
|                        | \(E^b\) | 70.0693 | 175.9788 | 330.1368 | 533.3216 |
|                        | \(E^e\) | 176.2699 | 330.4933 | 533.0876 |
|                        | \(E^f\) | 176.4441 | 330.8253 | 533.5611 |
Table 16. Comparison of the present calculations on the variational calculation of the excitation energies of the doubly excited states \((n\ell^2) \, ^1 \text{D}^\ell \,(n = 2 - 5)\) of the He-like systems with some theoretical results available in the literature consulted for \(Z = 2 - 5\). All the results are expressed in eV.

| States \((n\ell^2) \, ^1 \text{D}^\ell \,(n = 2 - 5)\) | \(Z\) | 2     | 3     | 4     | 5     |
|-----------------------------------------------|-----|-------|-------|-------|-------|
| \(3\ell^2 \, ^1 \text{G}^\ell\)              | \(E\) | 70.3444 | 176.2471 | 330.8215 | 533.7867 |
|                                              | \(E\) | 70.6245 | 176.9557 | 331.6960 | 534.8128 |
|                                              | \(E\) | 71.0544 | 177.3529 | 332.0144 | 535.0495 |
|                                              | \(E\) | 70.5238 | 176.9421 | 331.7477 | 534.9298 |
|                                              | \(E\) | 74.0939 | 185.7314 | 348.5466 | 562.3881 |
| \(4\ell^2 \, ^1 \text{G}^\ell\)              | \(E\) | 74.3089 | 186.0362 | 348.7685 | 562.5167 |
|                                              | \(E\) | 73.7021 | 185.5789 | 348.2569 | 561.9398 |
|                                              | \(E\) | 75.8420 | 190.1429 | 356.7827 | 575.6688 |
|                                              | \(E\) | 75.9470 | 190.2838 | 356.8475 | 575.6543 |
|                                              | \(E\) | 75.6667 | 189.8185 | 358.3822 | 575.0611 |
| \(5\ell^2 \, ^1 \text{G}^\ell\)              | \(E\) | 76.7975 | 192.5498 | 361.2720 | 582.9034 |
|                                              | \(E\) | 76.8667 | 192.6376 | 361.3047 | 582.8789 |
| \(6\ell^2 \, ^1 \text{G}^\ell\)              | \(E\) | 77.3770 | 194.0067 | 363.9872 | 587.2765 |
|                                              | \(E\) | 77.4273 | 194.0717 | 364.0150 | 587.2600 |

*Present work; aBachau et al. [19]; bRoy et al. [18]; cRay and Mukherjee [23].

with results obtained by the authors cited in Tables 14-16. Overall, we find a good agreement between our results and those of these authors. For all the states studied, the results obtained are in good agreement with the theoretical results we have consulted. The small difference noted between our results and those of the authors mentioned above is explained by the used method and the choice of the correlated wavefunction. The actual results presented in these different tables sufficiently show the good agreements between the current calculations and the different \textit{ab-initio} results for the doubly excited states \((n\ell^2) \, ^5 \text{S}^\ell\), \((np\ell^2) \, ^1 \text{D}^\ell\), \((n\ell^2) \, ^1 \text{G}^\ell\)
\(^1\!G^\prime, (n^f) \ ^1\!I^\prime, (n^g) \ ^1\!K^\prime, \) and \((n^h) \ ^1\!M^\prime\) of the He-like ions up to \(Z = 10\). This very good agreement sufficiently justifies the validity of the variational procedure of the SCUNC method to give the precise values obtained directly from an analytical expression, unlike all the \textit{ab-initio} methods cited in this document. Furthermore, the results quoted up to \(n = 20\) in this work may be interesting for future experimental and theoretical studies in the doubly excited states \((n^f) \ ^1\!L^\prime\). In summary, the manuscript reports on new calculations for key atomic-structure parameters of important fundamental few-body systems (helium and helium-like ions). While not allowing more precision tests of physics due to the neglect of relativistic, spin, and QED effects, such results can still be helpful in the future development of theories to describe more complex atoms, or may be further developed to study the time-dependent evolution of atoms in external \textit{(e.g. laser)} fields.

4. Conclusion

In this paper, the total energies and excitation energies of the doubly excited \((n^s) \ ^1\!S^\prime, (n^p) \ ^1\!D^\prime, (n^d) \ ^1\!G^\prime, (n^f) \ ^1\!I^\prime, (n^g) \ ^1\!K^\prime, \) and \((n^h) \ ^1\!M^\prime\) states of helium-like ions up to \(Z = 10\) are reported. These energies are calculated in the framework of the variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism. In this present work, a new wavefunction correlated to Hylleraas-type adapted to the correct description of electron-electron correlation phenomena in the \((n^f)\) doubly excited states of helium-like systems has been constructed. Our results for total energies and the excitation energies are in good agreement with the values cited in the experimental and theoretical literature. Furthermore, for \(n > 10\), no theoretical and experimental values from the literature are available for direct comparison. The good precision obtained in this work underlines that the results quoted up to \(n = 20\) in this work may be interesting for future experimental and theoretical studies in the doubly excited states \((n^f) \ ^1\!L^\prime\). The results presented in this paper show that it is therefore possible to perform an analytical calculation of the total energies of the \((n^f)\) doubly excited states for helium-like ions, without having to resort to excessively complicated calculations or a computer program.

Conflicts of Interest

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

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