Abstract — In this paper we present accurate calculated data of the energy levels of the $1snn^03L^s$ states ($l = s, p, d; n = 2 – 10$) of helium and heliumlike ions up to $Z = 12$ using the variational approach of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism. These calculations are performed by solving the time-independent Schrödinger equation using a new explicitly correlated wave function. A thorough comparison with theoretical predictions available in the literature for the energy levels of the singly excited $1sn^1S^o$, $1snp^1P^o$ and $1snd^3D^o$ Rydberg series is performed. Most of the tabulated results are generally in good agreement with the available reference data, confirming the reliability of our results. SCUNC predictions up to $n = 10$ may provide reliable atomic data for related experiments in the future.

Keywords—Energy Level, Excited States, Helium-Like Ions, Hylleraas Type Wave Function, Screening Constant by Unit Nuclear Charge (SCUNC).

I. INTRODUCTION

The present paper is a continuation of the work [1]-[3] where the energy levels of doubly excited states of helium-like ions were presented. The calculations in [1]-[3] were performed in the framework of the variational approach to the Screening Constant by Unit Nuclear Charge (SCUNC) formalism using new explicitly correlated wave functions.

Investigations of excited states in two-electron atomic systems have not only contributed to a better understanding of the dynamics of electronic correlations in multi-electron atomic systems, but in addition, these studies have provided a better understanding of the nature of ionization mechanisms in two and three-electron atomic systems. Indeed, the studies of multi-electron atomic systems constitute an irreplaceable tool for the development not only of new theoretical methods [4], [5] but also for the implementation of new experimental methods allowing a better understanding of the excitation and de-excitation processes of complex atomic systems on the one hand, and on the other hand, the detailed knowledge of the energy levels of the different excited states of highly charged ions is necessary to model the spectra of high-temperature astrophysical sources, tokamaks, and laser-generated plasma.

However on the experimental side, it should be noted that systematic experiments on the study of excited states were carried out from 1960 onwards with the development of synchrotron radiation which allowed Madden and Codling [6], [7] to carry out photoabsorption experiments in the far ultraviolet on various rare gases. Today, these studies of the properties of excited states concern very diverse fields of application in modern physics.

On the theoretical level, the study of the excited states of the helium atom and its isoelectronic series has been the subject of several theoretical approaches [8]-[11]. Thus, several studies are currently focused on the calculation of the energy levels of the ground state and doubly excited states of helium and heliumlike ions in relation to the importance of electronic correlations.

Although a lot of effort has been made in the last few years in the development of several theoretical methods for the description of atomic systems with more than two electrons, there is still room for further studies in this field in order to test new theoretical methods that can contribute to a better understanding of the phenomena of electronic correlations through a simple mathematical formalism. It is in this context that the present work is situated. Thus, in this paper, we focus only on the calculations of the single excitation energy levels of helium-like ions up to $Z = 12$ for ($1snl$) $^{1,3}L^s$ configurations.

Our goal in this present work is twofold, first it is to present accurate calculations of the energy levels of singly excited $1snl$ $^{1,3}L$ states of helium-like ions, and second it is to extend the existing calculations to highly excited levels ($n \leq 10$) which are useful data for the NIST database. For this purpose, we use the...
variational approach of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism and an explicitly correlated test wave function.

The SCUNC method [1]-[3] is very suitable for describing excited states of two-electron atomic systems. This calculation method is a combination of both perturbation theory and the variational Ritz method. It allows expressing analytically the resonance energies of the ground state and the different excited states of atomic systems with more than two electrons.

The present paper is organized as follows. In section II, we briefly present the theoretical method used in this work. In section III, our calculated results for the energy levels of singly excited 1snl states of two-electron atomic systems with Z ≤ 12 are tabulated and analyzed in detail, followed by a comparison with previous results. Conclusions and some perspectives for future work are summarized in section IV.

II. THEORY AND CALCULATIONS

A. Hamiltonian and Wave Functions

The non-relativistic, time-independent Schrödinger equation that describes the motion of the two electrons in two-electron atomic systems is given by (1).

\[ \hat{H} \psi(r_1, r_2) = E \psi(r_1, r_2) \]  

where \( \hat{H} \) represents the Hamiltonian operator of the considered system, \( \psi(r_1, r_2) \) the trial wave function and \( E \) the associated energy.

The non-relativistic Hamiltonian of the heliumlike ions is (in atomic units) given in (2).

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

where \( r_{1,2} \) are the radial coordinates of two electrons and \( r_{12} = \left| r_1 - r_2 \right| \) is the relative distance between them.

In the present approach, the explicitly correlated two-electron wave function \( \psi(r_1, r_2) \) used is developed as (3).

\[ \psi(r_1, r_2) = \frac{1}{4\pi} \sum_{\nu=0}^{n-1} (n^2 r_0^2)^{\nu} \left[ 1 + (-1)^{S} C_0 r_{12} \right] \exp \left[ -\lambda (r_1 + r_2) \right] \]  

In this expression, \( n \) and \( l \) are respectively the principal and orbital quantum numbers of the electron-\( nl \), \( r_0 \) is the Bohr radius, \( S \) is the total spin, \( \lambda \) and \( C_0 \) are the variational parameters to be determined by minimizing the energy, \( Z \) is the nuclear charge, \( r_1 \) and \( r_2 \) are the coordinates of the electrons with respect to the nucleus.

From the theoretical viewpoint, the Hylleraas variational method is based on the Hylleraas and Undheim theorem [12] according to which, a good approximation of the energy eigenvalue \( E(\lambda, C_0) \) is obtained when the minima of the function \( \left( \partial^2 E(\lambda, C_0) / \partial \lambda \partial C_0 \right) = 0 \) 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 \( \lambda \) and \( C_0 \) can be determined by the (4) and (5).

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

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

In the framework of the Ritz’ variation principle, the energy \( E = \langle H \rangle \) is calculated with (6).
E = \langle H \rangle = \left\langle \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \right\rangle \tag{6}

In (6), the correlated wave functions are given by (3) and the Hamiltonian $H$ of the helium isoelectronic series in given by (2) in atomic units.

Furthermore, the closure relation represents the fact that $\{ \vec{r}_1, \vec{r}_2 \}$ are continuous bases in the space of the two – electron space, written as (7).

$$\iint dr_1 dr_2 |\vec{r}_1, \vec{r}_2\rangle \langle \vec{r}_1, \vec{r}_2| = 1$$

Using this relation, according to (6), we obtain (8).

$$E \times \iint dr_1 dr_2 \langle \psi | \vec{r}_1, \vec{r}_2 \rangle \times \langle \vec{r}_1, \vec{r}_2 | \psi \rangle = \iint dr_1 dr_2 \langle \psi | \vec{r}_1, \vec{r}_2 \rangle \hat{H} \langle \vec{r}_1, \vec{r}_2 | \psi \rangle$$

By developing this expression (8), we find (9).

$$E \times \iint dr_1 dr_2 \psi \times \psi^* = \iint dr_1 dr_2 \psi \hat{H} \psi^*$$

This expression (9) can be rewritten according to (10)

$$N \times E = \iint dr_1 dr_2 \psi \hat{H} \psi^*$$

In (10), $N$ represents the normalization constant given by expression (11)

$$N = \iint dr_1 dr_2 |\psi|^2$$

To make it easier to integrate (9), we operate the variable changes in elliptic coordinates by (12).

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

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

$$d\tau = d^3r_1d^3r_2 = 2\pi^2 (s^2 - t^2) u \, ds \, du \, dt$$

Using these elliptical coordinates, (14) is rewritten as follows:

$$N \times E = \int_0^\infty ds \int_0^u du \int_0^t dt \left\{ u (s^2 - t^2) \times \left[ \left( \frac{\partial \psi}{\partial s} \right)^2 + \left( \frac{\partial \psi}{\partial t} \right)^2 + \left( \frac{\partial \psi}{\partial u} \right)^2 \right] + 2 \left( \frac{\partial \psi}{\partial u} \right) \times \left[ s (u^2 - t^2) \times \frac{\partial \psi}{\partial s} + t (s^2 - u^2) \times \frac{\partial \psi}{\partial t} \right] - \psi^2 \times (4Zsu - s^2 + t^2) \right\}$$

(14)

With respect to the correlated wave functions given by expression (3), it is expressed as (15).

$$\psi = \frac{1}{4\pi} \sum_{\nu = 0}^{n-1} \left( n^2 r_0^2 \right)^\nu \left[ 1 + (-1)^S C_0 Z u \right] \exp \left( -\lambda s \right)$$

(15)

Furthermore, according to (12), the normalization constant is written in elliptic coordinates as (16).
\[ N = \int_{s}^{t} ds \int_{u}^{t} du \left( s^2 - t^2 \right) \times y^2 \]  

(16)

B. General Formalism of the SCUNC Method

In the framework of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism, total energies of the \( N'l'nl^{2S+1}L^\pi \) excited states are expressed in Rydberg (Ry) \([1]\) as (17).

\[ E\left(N'l',nl^{2S+1}L^\pi;Z\right) = -Z^2\left\{ \frac{1}{N^2} + \frac{1}{n^2}\left[ 1 - \beta\left(N'l',nl^{2S+1}L^\pi;Z\right) \right] \right\} \text{Ryd} \]  

(17)

In (17), \( N \) and \( n \) designate the principal quantum numbers of the inner and outer electrons, respectively, of helium and helium-like ions the \( \beta \)-parameters are screening constant by unit nuclear charge expanded in inverse powers of \( Z \) and given by (18).

\[ \beta\left(N'l',nl^{2S+1}L^\pi;Z\right) = \sum_{k=1}^{q} f_k \left( N'l',nl^{2S+1}L^\pi; \left( \frac{1}{Z} \right)^k \right) \]  

(18)

where \( f_k = f_k \left( N'l',nl^{2S+1}L^\pi \right) \) are screening constants.

For the singly excited states \((1snl)^{1,3}L\) of helium-like ions, \( N = 1 \) and \( l' = 0 \). Hence, the total energy (17) is written as (19).

\[ E\left(1snl;2S+1L^\pi;Z\right) = -Z^2\left\{ 1 + \frac{1}{n^2}\left[ 1 - \beta\left(1snl;2S+1L^\pi;Z;\lambda\right) \right] \right\} \text{Ryd} \]  

(19)

where \( \beta\left(1snl;2S+1L^\pi;Z;\lambda\right) \) is the screening constant by unit nuclear charge expressed as a function of the variational parameter \( \lambda \) evaluated variationally using a wave function.

In this work, this screening constant per unit nuclear charge is expressed in terms of the variational \( \lambda \) parameter as (20).

\[ \beta\left(1snl^{1,3}L,Z,\lambda\right) = \frac{\lambda}{Z} \left( 1 + \frac{L+1}{nL+(S+1)+3} \right) \]  

(20)

In this expression, \( n \) denotes the principal quantum number of the outer electron, \( L \) denotes the quantum state under consideration \((S, P, D,..)\), \( S \) with \((S = 0 \text{ or } 1) \) is the total spin of the atomic system and \( \lambda \) is the variational parameter.

In practice, the correct expression of this term is sought by iteration. We test expression after expression and we stop the iteration from the last expression which gives results as close as possible to the experimental and theoretical results available.

Substituting expressions (18) into (17), the energy levels of the \((1snl)^{1,3}L^\pi (l = s, p, d)\) singly excited states in the heliumlike ions are then expressed as follows (in Ryd).

\[ E\left(1snl^{1,3}L,\lambda,Z\right) = -Z^2\left\{ 1 + \frac{1}{n^2}\left[ 1 - \frac{\lambda}{Z^2}\left( 1 + \frac{L+1}{nL+(S+1)+3} \right)^2 \right]\right\} \]  

(21)

In (21), only the variational parameter \( \lambda \) is unknown. The details of the calculation of this parameter are well explained in our previous work [1]-[3]. It is (21) that we used to calculate the energy levels of the \( (1sns)^{1,3}S^0 \), \( (1snp)^{1,3}P^0 \) and \((1snl)^{1,3}D^\pi \) \((2 \leq n \leq 10)\) singly excited states of the heliumlike ions \((Z \leq 12)\) without any complex calculation program or code.
III. RESULTS AND DISCUSSIONS

The results obtained from the present calculations are reported in Tables I-VI and are compared with the results of other methods. All results are expressed in atomic units (a.u).

Table I shows the comparison of the present results concerning the calculation of the energy levels ($-E$) for the singly excited ($1sns$) $1S^e (n=2-5)$ states of the helium atom and helium-like ions with the very recent data obtained by Zhang et al. [13] who used explicitly correlated Hylleraas configuration-interaction wave functions in the framework of the Ritz variability principle. Comparison is also made with the results of the modified atomic orbital theory [14], the double sum method on the total hydrogen spectrum of the product of the radial integrals of Ivanov and Safronova calculations [15] and finally with the analytical calculations of Arias de Saavedra et al. [16]. Overall, we find very good agreement between the present SCUNC calculations and the previous results cited above. For all the states presented in this table and up to $Z = 12$ the energy differences between the SCUNC predictions and the results of the authors mentioned in this table never exceeded 0.09 a.u which shows the very good accuracy of our calculations.

In Table II, the present results on the calculation of the energy levels ($-E$) of the states ($1sns$) $3S^e, (n=2-5)$ of the variational approach of the screening constant by unit nuclear charge (SCUNC) formalism are compared with the recent values of Zhang et al. [13], with the results of Sakho [17], with the data of Ivanov and Safronova [4] and with the results of the analytical calculations of Arias de Saavedra et al. [16]. Here also, we note a very satisfactory agreement between our results and the results of the authors quoted above. In general our results concerning the energy levels of the singlet and simply excited triplet ($1sns$) $1S^e, 3S^e$ states of helium-like systems are in agreement with those of other authors using other theoretical or experimental methods. It should be mentioned that in this present work, the existing data for these two states were extended to the $n = 10$ level.

Table III shows a comparison between the present SCUNC calculations of the Rydberg series ($1snp$) $1p^0$ energy levels of He-like ions with the data of Zhang et al. [13], with the results of the modified atomic orbital theory of Sakho [14] and with the theoretical data of Ivanov and Safronova [15]. Here again, the agreements are very good since the deviations between our calculations and the data of the others cited in this table almost never exceeded 0.09 a.u up to $n = 5$ and up to $Z = 12$. For $n > 5$, no data is quoted in the literature consulted and our predictions for $n = 5$ recorded in Table III can therefore be good reference values for the ($1snp$) $1p^0$ singly excited states of He-like ions.

**TABLE I: COMPARISON OF THE PRESENT SCREENING CONSTANT BY UNIT NUCLEAR CHARGE (SCUNC) FOR ENERGY LEVELS ($-E$) OF RYDBERG SERIES ($1sns$) $1S^e (n=2-5)$ OF THE HELIUM-LIKE IONS FOR $Z = 2-12$ WITH OTHER THEORETICAL VALUES.**

| States         | Z | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|----------------|---|----|----|----|----|----|----|----|----|----|----|----|
| $1sns 1S^e$    | $\lambda$ | 1.629 | 1.629 | 3.244 | 4.100 | 4.559 | 5.205 | 6.299 | 6.931 | 7.730 | 8.700 | 9.190 |
| $-E^c$         | 2.131 | 5.037 | 9.145 | 14.516 | 21.237 | 29.164 | 38.223 | 48.654 | 60.290 | 73.129 | 87.351 |
| $-E^e$         | 2.146 | 5.041 | 9.185 | 14.579 | - | - | - | - | - | - | - |
| $1sns 3S^e$    | -$E^c$ | 2.146 | 5.042 | 9.192 | 14.590 | 21.237 | 29.135 | 38.283 | 48.681 | 60.329 | 73.227 | 87.374 |
| $-E^e$         | 2.151 | 5.044 | 9.187 | 14.580 | 21.224 | 29.043 | 38.260 | 48.653 | 60.296 | 73.189 | 87.333 |
| $1sns 5S^e$    | -$E^c$ | 2.146 | - | - | 21.222 | - | - | - | - | 60.295 | - | - |
| $-E^e$         | 2.061 | 4.744 | 8.518 | 13.409 | 19.453 | 26.590 | 34.787 | 44.147 | 54.600 | 66.143 | 78.855 |
| $1sns 3S^e$    | -$E^c$ | 2.061 | 4.734 | 8.517 | 13.412 | - | - | - | - | - | - |
| $-E^e$         | 2.061 | 4.736 | 8.522 | 13.420 | 19.428 | 26.547 | 34.778 | 44.120 | 54.573 | 66.136 | 78.811 |
| $1sns 3S^e$    | -$E^c$ | 2.061 | 4.733 | 8.517 | 13.412 | 19.418 | 26.535 | 34.763 | 44.102 | 54.552 | 66.114 | 78.786 |
| $-E^e$         | 2.061 | - | - | - | 19.418 | - | - | - | - | - | - |
| $1sns 5S^e$    | -$E^c$ | 2.036 | 4.640 | 8.295 | 13.016 | 18.823 | 25.683 | 33.576 | 42.561 | 52.598 | 63.687 | 75.869 |
| $-E^e$         | 2.034 | 4.630 | 8.289 | 13.010 | - | - | - | - | - | - | - |
| $1sns 3S^e$    | -$E^c$ | 2.032 | 4.629 | 8.288 | 13.010 | 18.836 | 25.642 | 33.551 | 42.523 | 52.558 | 63.655 | 75.814 |
| $-E^e$         | 2.030 | 4.630 | 8.288 | 13.010 | 18.791 | 25.640 | 33.551 | 42.520 | 52.553 | 63.650 | 75.809 |
| $1sns 5S^e$    | -$E^c$ | 2.024 | 4.591 | 8.191 | 12.833 | 18.530 | 25.280 | 33.013 | 41.824 | 51.668 | 62.546 | 74.483 |
| $-E^e$         | 2.021 | 4.582 | 8.184 | 12.825 | - | - | - | - | - | - | - |

*present work.
*Ref. [13]
*Ref. [14]
*Ref. [15]
*Ref. [16]
In Table IV, we compare our present SCUNC results for singly excited (1snp) 1p0 triplet states with the previous results of Zhang et al. [13], Sakho [17] and Ivanov and Safronova [4]. For these states too, we note an excellent agreement between our present predictions and the results of the other methods cited. It is worth mentioning that up to n = 5 and up to Z = 12, the absolute energy deviations of our results from the cited reference values never exceed 0.09 a.u., which sufficiently justifies the very high accuracy of our calculations and the adequacy of the present formalism applied to the calculation of excited state levels of multiply charged atomic systems.

In Table V and Table VI, the energy levels of singlet and triplet (1snd) 1,3D0 singly excited states are compared with those obtained by Zhang et al. [13] using explicitly correlated Hylleraas configuration-interaction wave functions within the framework of the Ritz variability principle, by Sakho [14], [17] with the modified atomic orbital theory (MAOT) and by Ivanov and Safronova [4], [15] applying the doublesum method on the total hydrogen spectrum of the product of radial integrals. This comparison shows that the present calculations of the variational approach of the SCUNC formalism are in very good agreement with the results of the other methods and with a very high accuracy up to Z = 12.

| States1sns3S0 | Z | λ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|--------------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -            | Ep | 2.069 | 4.772 | 8.572 | 13.486 | 19.471 | 26.611 | 34.813 | 44.176 | 54.633 | 66.180 | 78.894 |
| -            | Eν2 | 2.069 | 4.752 | 8.547 | 13.453 | - | - | - | - | - | - | - | - | - |
| 1s2s 3S0     | Ep | 2.069 | 4.754 | 8.550 | 13.457 | 19.475 | 26.604 | 34.845 | 44.196 | 54.659 | 66.233 | 78.918 |
| -            | Eν2 | 2.067 | 4.751 | 8.546 | 13.453 | 19.470 | 26.599 | 34.838 | 44.189 | 54.651 | 66.224 | 78.908 |
| -            | Eν2 | 2.069 | - | - | 19.470 | - | - | - | - | 54.651 | - | - | - | - |
| 1s4s 3S0     | Ep | 2.040 | 4.654 | 8.324 | 13.057 | 18.831 | 25.692 | 33.587 | 42.574 | 52.612 | 63.703 | 75.886 |
| -            | Eν2 | 2.037 | 4.637 | 8.300 | 13.026 | 18.808 | 25.658 | 33.571 | 42.547 | 52.584 | 63.685 | 75.848 |
| -            | Eν2 | 2.031 | 4.632 | 8.295 | 13.020 | 18.815 | 25.666 | 33.579 | 42.555 | 52.593 | 63.694 | 75.858 |
| -            | Eν2 | 2.036 | 4.637 | 8.300 | 13.026 | - | - | - | - | - | - | - | - | - |
| 1s5s 3S0     | Ep | 2.026 | 4.599 | 8.208 | 12.858 | 18.534 | 25.265 | 33.019 | 41.830 | 51.675 | 62.554 | 74.491 |
| -            | Eν2 | 2.023 | 4.586 | 8.190 | 12.833 | - | - | - | - | - | - | - | - | - |
| 1s6s 3S0     | Ep | 2.018 | 4.569 | 8.145 | 12.750 | 18.372 | 25.033 | 32.709 | 41.426 | 51.166 | 61.929 | 73.733 |
| -            | Eν2 | 2.014 | 4.551 | 8.107 | 12.684 | 18.274 | 24.892 | 32.522 | 41.181 | 50.858 | 61.551 | 73.275 |
| 1s7s 3S0     | Ep | 2.010 | 4.539 | 8.082 | 12.641 | 18.210 | 24.801 | 32.400 | 41.022 | 50.658 | 61.306 | 72.977 |
| -            | Eν2 | 2.008 | 4.531 | 8.065 | 12.612 | 18.166 | 24.738 | 32.317 | 40.913 | 50.520 | 61.138 | 72.773 |
| 1s8s 3S0     | Ep | 2.007 | 4.525 | 8.053 | 12.591 | 18.135 | 24.693 | 32.257 | 40.835 | 50.422 | 61.017 | 72.627 |

1Present work.
2Ref. [13]
3Ref. [17]
4Ref. [4]
5Ref. [16]
### TABLE III: COMPARISON OF THE PRESENT SCREENING CONSTANT BY UNIT NUCLEAR CHARGE (SCUNC) FOR ENERGY LEVELS (–E) OF RYDBERG SERIES (1snp) 1pE (N = 2 – 5) OF THE HELIUM-LIKE IONS FOR Z = 2 – 12 WITH OTHER THEORETICAL VALUES.

| States 1snp 1pE | Z  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|----------------|----|----|----|----|----|----|----|----|----|----|----|----|
|                | λ  |    |    |    |    |    |    |    |    |    |    |    |
| 1s2p 1pE       | -E | 2.111 | 4.990 | 9.102 | 14.477 | 21.090 | 28.920 | 38.069 | 48.445 | 60.054 | 72.994 | 87.017 |
|                | E  | 2.124 | 4.993 | 9.111 | 14.477 |    |    |    |    |    |    |    |
| 1s3p 1pE       | -E | 2.055 | 4.724 | 8.499 | 13.391 | 19.389 | 26.484 | 34.720 | 44.057 | 54.498 | 66.985 | 78.710 |
|                | E  | 2.055 | 4.720 | 8.496 | 13.383 |    |    |    |    |    |    |    |
| 1s4p 1pE       | -E | 2.033 | 4.629 | 8.285 | 12.999 | 18.788 | 25.624 | 33.539 | 42.511 | 52.542 | 63.654 | 75.789 |
|                | E  | 2.031 | 4.624 | 8.280 | 12.997 |    |    |    |    |    |    |    |

*present work.
*Ref. [13]
*Ref. [14]
*Ref. [15]

### TABLE IV: COMPARISON OF THE PRESENT SCREENING CONSTANT BY UNIT NUCLEAR CHARGE (SCUNC) FOR ENERGY LEVELS (–E) OF RYDBERG SERIES (1snp) 1pE (N = 2 – 5) OF THE HELIUM-LIKE IONS FOR Z = 2 – 12 WITH OTHER THEORETICAL VALUES.

| States 1snp 1pE | Z  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|----------------|----|----|----|----|----|----|----|----|----|----|----|----|
|                | λ  |    |    |    |    |    |    |    |    |    |    |    |
| 1s2p 1pE       | -E | 2.119 | 5.021 | 9.133 | 14.521 | 21.126 | 29.053 | 38.104 | 48.521 | 60.140 | 73.004 | 87.110 |
|                | E  | 2.133 | 5.028 | 9.175 | 14.573 |    |    |    |    |    |    |    |
| 1s3p 1pE       | -E | 2.056 | 4.737 | 8.513 | 13.411 | 19.405 | 26.542 | 34.735 | 44.090 | 54.535 | 66.089 | 78.751 |
|                | E  | 2.058 | 4.730 | 8.515 | 13.410 |    |    |    |    |    |    |    |
| 1s4p 1pE       | -E | 2.033 | 4.636 | 8.293 | 13.018 | 18.797 | 25.657 | 33.549 | 42.530 | 52.564 | 63.658 | 75.813 |
|                | E  | 2.032 | 4.628 | 8.287 | 13.008 |    |    |    |    |    |    |    |
| 1s5p 1pE       | -E | 2.022 | 4.589 | 8.189 | 12.834 | 18.514 | 25.245 | 32.996 | 41.805 | 51.647 | 62.528 | 74.449 |
|                | E  | 2.021 | 4.582 | 8.183 | 12.825 |    |    |    |    |    |    |    |

*present work.
*Ref. [13]
*Ref. [17]
*Ref. [4]

### TABLE V: COMPARISON OF THE PRESENT SCREENING CONSTANT BY UNIT NUCLEAR CHARGE (SCUNC) FOR ENERGY LEVELS (–E) OF RYDBERG SERIES (1snd) 1D (N = 3 – 5) OF THE HELIUM-LIKE IONS FOR Z = 2 – 12 WITH OTHER THEORETICAL VALUES.

| States 1snd 1D | Z  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|---------------|----|----|----|----|----|----|----|----|----|----|----|----|
|               | λ  |    |    |    |    |    |    |    |    |    |    |    |
| 1s3d 1D       | -E | 2.051 | 4.722 | 8.500 | 13.380 | 19.389 | 26.500 | 34.684 | 44.056 | 54.500 | 66.056 | 78.724 |
|               | E  | 2.056 | 4.722 | 8.500 | 13.389 |    |    |    |    |    |    |    |
| 1s4d 1D       | -E | 2.032 | 4.631 | 8.290 | 13.007 | 18.797 | 25.643 | 33.532 | 42.524 | 52.559 | 63.656 | 75.816 |
|               | E  | 2.031 | 4.625 | 8.281 | 13.000 |    |    |    |    |    |    |    |
| 1s5d 1D       | -E | 2.022 | 4.587 | 8.190 | 12.831 | 18.517 | 25.241 | 32.991 | 41.807 | 51.651 | 62.534 | 74.459 |
|               | E  | 2.020 | 4.580 | 8.180 | 12.820 |    |    |    |    |    |    |    |

*Ref. [13]
*Ref. [17]
*Ref. [4]
research on the excited states of two isoelectronic series of very high nuclear charge Z have also been demonstrated. The many precise results we have presented in this paper, sufficiently justify once again the validity of the present approach of the SCUNC (Screening Constant by Unit Nuclear Charge) formalism.

Overall, the very good agreements noted between the present SCUNC calculations of the energy levels of singular and triplet (1snp) 1,3Lz singly excited states of helium-like ions (Z = 12) and the various very accurate \textit{ab-initio} results we have presented in this paper, sufficiently justify once again the validity of the present approach of the SCUNC (Screening Constant by Unit Nuclear Charge) formalism as applied to the study of singular and doubly excited states of two-electron atomic systems. It is worth mentioning that the calculations are directly obtained from simple analytical formulas, contrary to other \textit{ab-initio} methods which usually require sometimes complicated computer programs or complex calculation codes.

### IV. Conclusion

In this paper, the variational approach of the screening constant per unit nuclear charge (SCUNC) formalism has been successfully applied to the calculation of the energy levels of the excited states (1snl) 1,3Lz (l = s, p, d) of helium and helium-like ions of nuclear charge Z ≤ 12. These calculations are performed using explicitly correlated special-form wave functions by solving the time-independent Schrödinger equation. In general, the present predictions of the SCUNC method are in good agreement with existing theoretical data. The possibilities of using the variational approach of the SCUNC formalism for the calculation of energy levels in the singly excited 1sns 1,3Sx, 1snp 1,3P0 and 1snd 1,3Dx states of helium and its iso electronic series of very high nuclear charge Z have also been demonstrated. The many precise results listed in tabular form in this paper once again show the merit of the variational approach of the screening constant per unit nuclear charge method applied to the calculation of the excited state energies of atomic systems with two electrons. We believe that this precise data presented in this paper will be of great importance to the community of atomic physicists in connection with future experimental and/or theoretical research on the excited states of two-electron atoms in dense quantum plasmas.

**Funding**

The author did not receive any financial support from any funding agencies.
CONFLICT OF INTEREST

Authors declare that they do not have any conflict of interest.

REFERENCES

[1] Gning MT, Sakho I, Sow M. Calculations Energy of the (n²) 1L⁺ Doubly Excited States of Two-Electron Systems via the Screening Constant by Unit Nuclear Charge Formalism. Journal of Modern Physics, 2020 November 25; 11 (11): 1891-1910.https://doi.org/10.4236/jmp.2020.1111118.

[2] Gning MT, Sakho I, Faye M, Sow M, Diop B, Badiane J K, Ba D, Diao Al. Variational Calculations of Energies of the (2snl) 1L⁺ and (2pnl) 1L⁺ Doubly Excited States in Two-Electron Systems Applying the Screening Constant per Unit Nuclear Charge. Journal of Modern Physics, 2021 February 26; 12(3): 328-352.https://doi.org/10.4236/jmp.2021.123024.

[3] Gning MT, Sakho I. Doubly-Excited 1S⁺, 1P⁺, 1D⁺, 1P² and 1G⁺ Resonances States of Two-Electron Atoms below the N = 3 – 8 Hydrogenic Thresholds. International Journal of Physics, 2022January 23; 10 (1): 23 - 48.DOI: 10.12691/ijp-10-1-2.

[4] Ivanov IA, Safronova UL. Calculation of the correlation part of the energy to two-electron systems. Optics and Spectroscopy, 1993 September; 75 (3): 506-516.

[5] Zhou Z, Chu C. Spin-dependent localized Hartree-Fock density-functional calculation of singly, doubly and triply excited and Rydberg states of He and Li-like ions. Physical Review A2005 February 28; 71(2):022513.DOI: https://doi.org/10.1103/PhysRevA.71.022513.

[6] Madden RP, Codling K. New Autoionizing Atomic Energy Levels in He, Ne, and Ar. Physical Review Letters, 1963;10(12): 516. Doi:https://doi.org/10.1103/PhysRevLett.10.516.

[7] Madden RP, Codling K. Two-Electron Excitation States in Helium. The Astrophysical Journal,1965;141, 364-375.https://doi.org/10.1086/148132.

[8] Balashov VV, Grishanova SI, Kruglova IM, Senashenko VS. Optics and Spectroscopy, 1970; T28: 858-868.

[9] Macek JH. Proceedings of the Physical Society of London,1967 92: 351.

[10] Ray D, Mukherjee PK. Doubly excited 'S', 'D' and 'G' states of He, Li, Be²⁺ and B⁴⁺. Journal of Physics B: Atomic, Molecular and Optical Physics, 1991 24 (6): 1241. DOI:https://doi.org/10.1088/0953-4075/24/6/013.

[11] Balashev E, Combes JM. Spectral properties of many-body Schrodinger operators with dilatation-analytic interactions. Communications in Mathematical Physics, 1971; December 22: 280-294. DOI: https://doi.org/10.1007/BF01877511.

[12] Hylleraas EA, Undheim B. Numerische Berechnung der 2S-Terme von orthound Par-Helium.Zeitschrift für Physik,1930;65:759 -772.https://doi.org/10.1007/BF01397263.

[13] Zhang YZ, Jiao LG, Liu F, Liu AH, Ho YK. Energy levels of ground and singly excited states of two-electron atoms in dense quantum plasma. Atomic Data and Nuclear Data Tables, 2021; 40:101420. https://doi.org/10.1016/j.adt.2021.101420.

[14] Sakho I. A Modification of Atomic Orbital Theory and Its Application to (1sln) L⁺ and (n²) L⁺ Excited States of He-Like Ions. Journal of Atomic and Molecular Sciences, 2010;1:103-117. DOI:10.4208/jams.022510.031010a.

[15] Ivanov AI, Safronova IU. Calculation of the Correlation Part of the Energy of Two-Electron Systems. Optics and Spectroscopy, 1993; 75: 298-304.

[16] Arias de Saavedra F, Porras I, Bueda E, Gilvez JF, Porras I. Spatial generalizations of Kato’s cusp condition for two-electron atoms with correlations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995;28: 3132.DOI:10.1088/0953-4075/29/17/007.

[17] Sakho I. Modified Atomic Orbital Calculations for (1sln) L⁺and ±(1,0)s⁻¹S⁺ Excited States of He Isoelectronic Sequence. Journal of Atomic and Molecular Sciences, 2010; 1: 224-242 (2010). DOI: 10.4208/jams.042710.051510a.