J. At. Mol. Sci.
doi: 10.4208/jams.062910.072810a

Vol. **2**, No. 1, pp. 20-42
February 2011

Energy resonances for $^1P^o$, $^1D^e$, $^1F^o$, $^1G^e$, and $^1H^o$ autoionizing states of the helium isoelectronic series below the $n=2$–4 hydrogenic thresholds

I. Sakho[*]

*UFR Sciences and Technologies, Department of Physics, University of Ziguinchor,
Ziguinchor, Senegal*

Received 29 June 2010; Accepted (in revised version) 28 July 2010

Abstract. General formalism of special form of Hylleraas correlated wave functions (SFHCWF) is demonstrated in this paper. The adequacy of the SFHCWF in the description as well as of the singlet than of the triplet excited states of two electron systems is also presented in this work. Application of SFHCWF to the calculations of doubly excited $nlnl'$ states $(n=2–4)$ in the helium-like ions is done, using the screening constant by unit nuclear charge method in the framework of a variational procedure. Comparison with various available theoretical and experimental literature values indicates a good agreement.

PACS: 31.15.p, 31.15.Ar, 31.25.Jf

Key words: energy resonances, helium isoelectronic series, special form of Hylleraas correlated wave functions, screening constant by unit nuclear charge, He-like ions

1 Introduction

The most suitable approached method used for the treatment of the ground state of two electron systems is the Ritz variational principal which has been first applied to the helium atom by Kellner [1] and with even great success by Hylleraas [2]. Since the early experiment of Madden and Codling [3] and others [4] and theoretical explanation of Cooper, Fano and Prats [5], doubly-excited states (DES) of the helium-like ions have been the intention of several studies. Besides, higher-energy Rydberg envelopes contain doubly-excited states which are generally labelled in the usual spectroscopic notation $(Nl,nl')^{2S+1}\,L^{\pi}$ with $n=N$, $N+1,\cdots$ [6]. In these notations, N and n denote respectively the principal quantum numbers of the inner and the outer electron, l and l' there respective orbital quantum numbers, S the total spin, L the total angular momentum and π the parity of the system.

---

[*] Corresponding author. *Email address:* `aminafatima_sakho@yahoo.fr` (I. Sakho)

Investigations of DES in two electron systems are of interest in spectroscopic diagnostic in connexion with the understanding of collisional and radiational processes taking place in hot astrophysical and laboratory plasmas [7]. For autoionizing states in the helium isoelectronic series, many computational methods are employed. Among these methods are, the computing double sum method over the complete hydrogen spectrum [8], the complex-coordinate rotation [9–12], the density functional theory [24], the Feshbach-projection method [14], the screening constant by unit nuclear charge (SCUNC) method [15–17] (to name a few). Special type of trial wave functions combining Hylleraas and incomplete hydrogenic wave functions have also been used in the computations of energies for doubly excited states of two electron systems [18–21]. But in these studies, the special form of Hylleraas correlated wave functions (SFHCWF) used by Biaye and co-workers [18–21], has been constructed by an iterative procedure.

In this paper, we present the general mathematical formalism that leads to the construction of such special wave functions. The adequacy of the SFHCWF in the description as well as of the singlet than of the triplet excited states of two electron systems is also presented. Besides, using the SCUNC- method, we apply SFHCWF in the calculations of $2s2p\,^1P^o$, $3s3p\,^1P^o$, $4s4p\,^1P^o$, $3s3d\,^1D^e$, $4s4d\,^1D^e$, $4s4f\,^1F^o$, $4p4d\,^1F^o$, $4p4f\,^1G^e$ and $4d4f\,^1H^o$ DES in He-like ions up to $Z=10$.

The advantages of the SCUNC method are connected with the possibilities to investigate autoionizing states in two-electron systems using either a variational or a semi-empirical procedure. Comparison of the results obtained with various theoretical other results is made. Discussions between the two procedures (semi-empirical and variational) of the SCUNC method are also made. In Section 2, we present the theoretical procedure adopted in this work. In Section 3, we present and discuss the results obtained, compared to available theoretical and experimental literature values.

2 SfHCWF for doubly excited states of two electron systems

For the ground state of two electron systems, the Hylleraas wave function is in the form

$$\Phi_{jkm}(\vec{r_1},\vec{r_2})=(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m\exp-\lambda(r_1+r_2). \tag{1}$$

In this expression, $\vec{r_1}$ and $\vec{r_2}$ denote the positions of the two electrons, r_1 and r_2 are used respectively for $|\vec{r_1}|$ and $|\vec{r_2}|$, j, k, m are Hylleraas parameters satisfying the double condition ($j,\ k,\ m\geq 0$) and $j+k+m\leq 3$, λ represents a coefficient given by: $\lambda=Z/\alpha r_0$, where Z, α and r_0 denote respectively the nuclear charge number, the variational parameter and the Bohr's radius. The set of the parameters (j, k, m) define the basis states and then give their dimension D. From the theoretical viewpoint, the Hylleraas variational method is based on the Hylleraas and Undheim theorem [22] according to which, a good approximation of the energy eigenvalue $E(\alpha)$ is obtained when the minima of the function ($\mathrm{d}E(\alpha)/\mathrm{d}\alpha=0$) converge with increasing values of the dimension D of the basis states and when the function exhibit a plateau. In the Hylleraas wave function, the angular part corresponding to the spherical harmonic $Y(\Theta,\varphi)$ is determined by the cosinus of the angle θ_{12} between the direction of the vector positions $\vec{r_1}$ and $\vec{r_2}$ as shown in the following expression

$$|\vec{r_1}-\vec{r_2}|=\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_{12}}.$$

On the other hand, in the Hylleraas variational method, the Hamiltonian operator relative to the two electron systems is shared in three terms as follows

$$H=T+C+W.$$

In this above decomposition, T denotes the kinetic energy operator of the two electrons, C is the Coulomb potential energy operator between the atomic nucleus and the two electrons and W represents the Coulomb interaction energy operator between the two electrons. These operators are given respectively by

$$\begin{aligned} T&=-\frac{\hbar^2}{2m}(\Delta_1+\Delta_2),\\ C&=-\frac{Ze^2}{r_1}-\frac{Ze^2}{r_2},\\ W&=\frac{e^2}{r_{12}}=\frac{e^2}{|\vec{r_1}-\vec{r_2}|}. \end{aligned}$$

In the framework of the Hylleraas method, the total ground state energy E is written as the sum of the average values of these three terms

$$\langle H\rangle=\langle T\rangle+\langle C\rangle+\langle W\rangle.$$

For an operator A, the average value $\langle A\rangle$ in the non normalized ground state wave function given by Eq. (1) is in the form

$$\langle A\rangle=\frac{\langle\Phi_{jkm}|A|\Phi_{j'k'm'}\rangle}{\langle\Phi_{jkm}|\Phi_{j'k'm'}\rangle}=\frac{\langle\Phi_{jkm}|A|\Phi_{j'k'm'}\rangle}{N_{JKM}},$$

where

$$N_{JKM}=\langle\Phi_{jkm}|\Phi_{j'k'm'}\rangle$$

denotes the matrix element of the normalisation constant. The parameters J, K, and M are equal respectively to: $J=j+j'$, $K=k+k'$, and $M=m+m'$. Using Eq. (1), we obtain

$$N_{JKM}=\iiint d^3r_1d^3r_2(r_1+r_2)^J(r_1-r_2)^K|\vec{r_1}-\vec{r_2}|^M\exp{-2\lambda(r_1+r_2)}.$$

In term of the matrix elements, the total ground state energy E satisfies the following relation

$$EN_{JKM}=T_{jkmj'k'm'}+C_{JKM}+W_{JKM}.$$

To facilitate the calculations of the above matrix elements, Hylleraas [2] used three distance coordinates defined as follows

$$v=(r_1+r_2),\;\; w=(r_1-r_2),\;\; u=\cos\theta_{12}.$$

By use of these variables, the matrix elements N_{JKM}, $T_{jkmj'k'm'}$, C_{JKM} and W_{JKM} are evaluated. One finds respectively

$$N_{JKM}=\frac{2\pi^2}{M+2}\left(\frac{1}{(K+1)}-\frac{1}{(K+3)}-\frac{1}{(K+M+3)}+\frac{1}{(K+M+5)}\right)(J+K+M+5)!\left(\frac{1}{2\lambda}\right)^{J+K+M+6},$$

$$W_{JKM}=e^2N_{JKM-1},$$

$$C_{JKM}=-\frac{8\pi^2Ze^2}{(M+2)}\left(\frac{1}{(K+1)}-\frac{1}{(K+M+3)}\right)(J+K+M+4)!\left(\frac{1}{2\lambda}\right)^{J+K+M+5},$$

$$\begin{aligned}T_{jkmj'k'm'}=\frac{\hbar^2}{2m}\Bigg(&2\Big(\lambda^2N_{JKM}-J\lambda N_{J-1,KM}+jj'N_{J-2,KM}+kk'N_{J,K-2,M}+mm'N_{J,K,M-2}\Big)\\&+\frac{1}{2}\Big(-M\lambda(C_{JKM}-C_{J,K+2,M-2})+(mj'+m'j)(C_{J-1,KM}-C_{J-1,K+2,M-2})\\&+(mk'+m'k)(C_{J+1,K,M-2}-C_{J-1,KM})\Big)\Bigg).\end{aligned}$$

These matrix elements with respect to the ground state of two electron systems are evaluated using a computer program. This permits to obtain the total ground state energy

$$E=\langle T\rangle+\langle C\rangle+\langle W\rangle.$$

The method has been applied successfully first by Hylleraas [2] in the ground state of the helium isoelectronic series. After, Biaye *et al.* [18–21] have extended the method to the calculations of energies for doubly excited stated of the helium atom and its isoelectronic sequence. But the wave functions combining Hylleraas and incomplete hydrogenic wave functions used by these authors have just been constructed by an iterative procedure. The form of the wave functions is considered as acceptable, if it permits to succeed at results in good agreement with other available experimental and theoretical results. Obviously, such a procedure could take a lot of time. To facilitate the construction of the special wave functions combining Hylleraas and incomplete hydrogenic wave functions, it is necessary to develop the general mathematical formalism that leads to the construction of such special wave functions. The first part of the present work is in this direction.

2.1 Incomplete hydrogenic wave functions for (nl^2) symmetric doubly excited states of the helium-like ions

For doubly excited states of type (nl^2), the correlated wave functions $\Psi_{jkmnl}(\vec{r_1},\vec{r_2})$ are constructed considering the product of incomplete radial hydrogenic wave functions $R_{nl}(r_1,r_2)$ by Hylleraas wave functions $\Phi_{jkmn}(\vec{r_1},\vec{r_2})$

$$\Psi_{jmknl}(\vec{r_1},\vec{r_2})=R_{nl}(r_1,r_2)x\Phi_{jkmn}(\vec{r_1},\vec{r_2}). \tag{2}$$

In this equation, $\Phi_{jkmn}(\vec{r_1},\vec{r_2})$ is given by Eq. (1) where the λ parameter for excited states is in the form $\lambda = Z/\alpha r_0 n$, n denotes the principal quantum number.

As far as the radial hydrogenic wave functions are concerned, they are in the general well knowing expression

$$R_{nl}(r) = \left(\left(\frac{2Z}{nr_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right)^{1/2} e^{-\frac{Zr}{nr_0}} \left(\frac{2Zr}{nr_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2Zr}{nr_0} \right). \tag{3}$$

In this formula, $L_{n+l}^{2l+1}(r)$ are Laguerre associated polynomials linked to the $L_{n+l}(r)$ − Laguerre polynomials by the Rodrigue's formula

$$L_n^k(r) = \frac{d^k}{dr^k} L_n(r),$$

where

$$L_n(r) = e^r \frac{d^n}{dr^n}(r^n e^{-r}).$$

On the other hand, complete hydrogenic wave functions are in the shape

$$\psi_{nl}(r,\theta,\varphi,s) = R_{nl}(r) \times Y_{lm}(\theta,\varphi) \times \phi(s).$$

In this equation, $R_{nl}(r)$ denotes the radial wave function given by Eq. (3), $Y_{lm}(\theta,\varphi)$ corresponds to the angular part of the wave function (also called spherical harmonics) and $\phi(s)$ designs the spin wave function. Ignoring both $Y_{lm}(\theta,\varphi)$ and $\phi(s)$, we obtained incomplete hydrogenic waves functions

$$\psi_{nl}(r) = R_{nl}(r).$$

Then, for the correlated waves functions $\psi_{nl}^{jkm}(r_1,r_2)$ we do the product

$$\psi_{nl}^{jkm}(r_1,r_2) = R_{nl}(r_1,r_2) \times \Phi_{jkm}(r_1,r_2) \times e^{\lambda(r_1+r_2)}. \tag{4}$$

The multiplication by the factor $(\exp\lambda(r_1+r_2))$ in the second term of the right hand side of Eq. (4) is justified by the fact that, each of the wave functions $(R_{nl}(r_1,r_2))$ and $\Phi_{jkm}(r_1,r_2)$ contains the exponential factor $\exp{-\lambda(r_1+r_2)}$. The main problem is to construct the incomplete hydrogenic wave functions $\psi_{nl}(r_1,r_2) = R_{nl}(r_1,r_2)$. In this purpose, we determine some radial hydrogenic wave functions in the particular cases of $1s$, $2s$, $2p$, $3s$ and $3p$ states. By use of general Eq. (3), we get

For 1s state, $R_{10}(r)=2\left(\frac{Z}{r_0}\right)^{3/2} e^{-\frac{Zr}{r_0}}$,

For 2s state, $R_{20}(r)=\frac{1}{\sqrt{2}}\left(\frac{Z}{r_0}\right)^{3/2}\left(1-\frac{Zr}{2r_0}\right)e^{-\frac{Zr}{2r_0}}$,

For 2p state, $R_{21}(r)=\frac{1}{2\sqrt{6}}\left(\frac{Z}{r_0}\right)^{5/2} re^{-\frac{Zr}{2r_0}}$,

For 3s state, $R_{30}(r)=\frac{2}{3\sqrt{3}}\left(\frac{Z}{r_0}\right)^{3/2}\left(1-\frac{2Zr}{3r_0}+\frac{2Z^2r^2}{27r_0^2}\right)e^{-\frac{Zr}{3r_0}}$,

For 3p state, $R_{31}(r)=\frac{8}{27\sqrt{6}}\left(\frac{Z}{r_0}\right)^{3/2}\left(\frac{Zr}{r_0}-\frac{Z^2r^2}{6r_0^2}\right)e^{-\frac{Zr}{3r_0}}$.

Besides, let us introduce the effective charge number Z^* defined by

$$Z^*=\frac{Z}{\alpha}. \tag{5}$$

where α is a variational parameter. Using Z^*, we construct non normalized incomplete radial wave functions considering the preceding hydrogenic waves functions

For 1s state, $R'_{10}(r)=e^{-\frac{Z^*r}{r_0}}$, (6a)

For 2s state, $R'_{20}(r)=\left(1-\frac{Z^*r}{2r_0}\right)e^{-\frac{Z^*r}{2r_0}}$, (6b)

For 2p state, $R'_{21}(r)=re^{-\frac{Z^*r}{2r_0}}$, (6c)

For 3s state, $R'_{30}(r)=\left(1-\frac{2Z^*r}{3r_0}+\frac{2Z^{*2}r^2}{27r_0^2}\right)e^{-\frac{Z^*r}{3r_0}}$, (6d)

For 3p state, $R'_{31}(r)=\left(\frac{Z^*r}{r_0}-\frac{Z^{*2}r^2}{6r_0^2}\right)e^{-\frac{Z^*r}{3r_0}}$. (6e)

On the other hand, the electron-electron correlation effects are taking into consideration by the parameters j, k and m of Hylleraas. We consider then, the incomplete hydrogenic wave functions given by Eq. (6) as wave functions of independent particles. Each electron is considered as interaction with the nucleus of effective charge Z^*. In this condition, if $\psi(\vec{r_1},\vec{r_2})$ is the wave function describing the global state of the two independent particles (1) and (2), in the basis $|\vec{r_1},\vec{r_2}\rangle$, we get

$$\psi(\vec{r_1},\vec{r_2})=\langle\vec{r_1},\vec{r_2}|\psi\rangle=\langle\vec{r_1}|\psi_1\rangle\langle\vec{r_2}|\psi_2\rangle=\psi_1(\vec{r_1})\times\psi_2(\vec{r_2}).$$

Besides, for identical particles (electrons here) the wave function can be written in the form

$$\psi'(\vec{r_1},\vec{r_2})=\psi_1(\vec{r_1})\times\psi_2(\vec{r_2})+\psi_1(\vec{r_2})\times\psi_2(\vec{r_1}).$$

This function is obtained by permuting the spatial coordinates r_1 and r_2 respectively of the two particles (1) and (2). Using these preceding equations, we construct the radial wave functions of the two electrons as follows

- For 1s state,

$$R_{10}(r_1,r_2)=R'_{10}(r_1)\times R'_{10}(r_2)=e^{-\frac{Z^*}{r_0}(r_1+r_2)}.$$

- For 2p state,

$$R'_{20}(r)=e^{-\frac{Z^*}{2r_0}r}-\frac{Z^*}{2r_0}re^{-\frac{Z^*}{2r_0}r}=R''_{20}(r)+R'''_{20}(r).$$

with

$$R''_{20}(r)=e^{-\frac{Z^*}{2r_0}r},\quad R'''_{20}(r)=-\frac{Z^*}{2r_0}re^{-\frac{Z^*}{2r_0}r}. \tag{7}$$

Let us put

$$R_{20}(r_1,r_2)=R''_{20}(r_1)\times R''_{20}(r_2)+R'''_{20}(r_1)\times R'''_{20}(r_2).$$

This, together with Eq. (7), gives

$$R_{20}(r_1,r_2)=e^{-\frac{Z^*}{2r_0}(r_1+r_2)}+\left(\frac{Z^*}{2r_0}\right)^2 r_1r_2\exp^{-\frac{Z^*}{2r_0}(r_1+r_2)},$$

which leads to

$$R_{20}(r_1,r_2)=\left(1+\left(\frac{Z^*}{2r_0}\right)^2 r_1r_2\right)e^{-\frac{Z^*}{2r_0}(r_1+r_2)}.$$

- For 2p state,

$$R_{21}(r_1,r_2)=R'_{21}(r_1)\times R'_{21}(r_2)=r_1r_2e^{-\frac{Z^*}{3r_0}(r_1+r_2)}.$$

- For 3s state,

$$R'_{30}(r)=e^{-\frac{Z^*r}{3r_0}}-\frac{2z^*r}{3r_0}e^{-\frac{Z^*r}{3r_0}}+\frac{2Z^{*2}r^2}{27r_0^2}e^{-\frac{Z^*r}{3r_0}}=R''_{30}(r)+R'''_{30}(r)+R''''_{30}(r).$$

with

$$R''_{30}(r)=e^{-\frac{Z^*}{3r_0}r},\ R'''_{30}(r)=-\frac{2Z^*r}{3r_0}e^{-\frac{Z^*}{3r_0}r},\ R''''_{30}(r)=\frac{2Z^{*2}r^2}{27r_0^2}e^{-\frac{Z^*}{3r_0}}. \tag{8}$$

Performing the following product

$$R_{30}(r_1,r_2)=R''_{30}\times R''_{30}(r_2)+R'''_{30}(r_1)\times R'''_{30}(r_2)+R''''_{30}(r_1)\times R''''_{30}(r_2),$$

we obtain using Eq. (8) that

$$R_{30}(r_1,r_2)=\left(1+\left(\frac{2Z^*}{3r_0}\right)^2 r_1r_2+\left(\frac{2Z^{*\,2}}{27r_0^2}\right)^2 r_1^2r_2^2\right)e^{-\frac{Z^*r}{3r_0}(r_1+r_2)}.$$

- For $3p$ state,

$$R'_{31}(r)=\frac{Z^*r}{r_0}e^{-\frac{Z^*r}{3r_0}}-\frac{Z^{*\,2}r^2}{6r_0^2}e^{-\frac{z^*r}{3r_0}}=R''_{31}(r)+R'''_{31}(r). \tag{9}$$

Let us put again

$$R_{31}(r_1,r_2)=R''_{31}(r_1)\times R''_{31}(r_2)+R'''_{31}(r_1)\times R'''_{31}(r_2).$$

That means using Eq. (9)

$$R_{31}(r_1,r_2)=\left(\left(\frac{Z^*}{r_0}\right)^2 r_1r_2+\left(\frac{Z^{*\,2}}{6r_0^2}\right)^2 r_1^2r_2^2\right)e^{-\frac{Z^*(r_1+r_2)}{3r_0}}.$$

Let us then summarize the equations to be used in the following study:

For $1s$ state, $R_{10}(r_1,r_2)=e^{-\frac{Z^*}{r_0}(r_1+r_2)}$, (10a)

For $2s$ state, $R_{20}(r_1,r_2)=\left(1+\left(\frac{Z^*}{2r_0}\right)^2 r_1r_2\right)e^{-\frac{Z^*}{2r_0}(r_1+r_2)}$, (10b)

For $3s$ state, $R_{30}(r_1,r_2)=\left(1+\left(\frac{2Z^*}{3r_0}\right)^2 r_1r_2+\left(\frac{2Z^{*\,2}}{27r_0^2}\right)^2 r_1^2r_2^2\right)e^{-\frac{Z^*}{3r_0}(r_1+r_2)}$, (10c)

For $2p$ state, $R_{21}(r_1,r_2)=r_1r_2e^{-\frac{Z^*}{3r_0}(r_1+r_2)}$, (10d)

For $3p$ state, $R_{31}(r_1,r_2)=\left(\left(\frac{Z^*}{r_0}\right)^2 r_1r_2+\left(\frac{Z^{*\,2}}{6r_0^2}\right)^2 r_1^2r_2^2\right)e^{-\frac{Z^*(r_1+r_2)}{3r_0}}$. (10e)

Let us then move on determining the general wave functions containing all the radial incomplete hydrogenic functions given by Eq. (10). In this purpose, we appeal to the general methodology of resolution of the Schrödinger's equation applied to the hydrogen-like ions. For the hydrogen-like ions, the Schrödinger's stationary equation is written in the well knowing form

$$\hat{H}\psi=E\psi,$$

where

$$\hat{H}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r_2}+\frac{2\partial}{r\partial r}\right)-\frac{Ze^2}{r}+\frac{\hat{l}^2}{2mr^2},\ \psi=R(r)\times Y(\theta,\phi).$$

For the stationary states, the square of the $\hat{l}^2$ – orbital angular momentum is given by

$$\hat{l}^2Y(\theta,\varphi)=\hbar^2l(l+1)Y(\theta,\varphi).$$

Using this result, the above Schrödinger's equation becomes

$$\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\frac{\partial\psi}{\partial r}+\left(\frac{q}{r}-\beta^2-\frac{l(l+1)}{r^2}\right)\psi=0 \tag{11}$$

with

$$q=\frac{2mZe^2}{\hbar^2}, \quad \beta=-\frac{2mE}{\hbar^2}. \tag{12}$$

Inserting $\psi=R(r)\times Y(\theta,\psi)$ into Eq. (11), we obtain the radial wave function equation

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dr}{dr}+\left(\frac{q}{r}-\beta^2-\frac{l(l+1)}{r^2}\right)R=0. \tag{13}$$

For the resolution of Eq. (13), the radial wave function R is generally written in the form [23]

$$R(r)=\frac{u(r)}{r}e^{-\beta r}. \tag{14}$$

Using this expression, Eq. (13) gives

$$\frac{d^2u}{dr^2}+\frac{2}{r}\frac{du}{dr}+\left(\frac{q}{r}-\beta^2-\frac{l(l+1)}{r^2}\right)u=0. \tag{15}$$

The solution of this differential equation is presented as follows

$$u(r)=\sum_{k=\gamma}^{\infty}a_k r^k. \tag{16}$$

By use of Eq. (16), Eq. (15) leads to the coefficients a_k after identification

$$\begin{aligned}&\gamma(\gamma+1)=l(l+1), && \text{for } k=\gamma.\\ &\big(k(k+1)-l(l+1)\big)a_{k+1}=(2\beta k-q)a_k, && \text{for } k\neq\gamma.\end{aligned}$$

The first equation gives the solution $\gamma=-l$ or $\gamma=(l+1)$.

The result $\gamma=-l$ is to be rejected as it leads to a wave function being infinite for $r\to 0$. This disagrees with the limits fixed to any wave function $\psi(r)$, solution of the Schrödinger's equation. In fact, $\psi(r)$ and its first spatial derivates must be finished, uniforms and continuous, even at the points of discontinuity of the potential function $U(r)$. Subsequently, the solution

$$\gamma=(l+1). \tag{17}$$

is conserved.

Besides, for the convergence of the series given by Eq. (16), the second solution above yields asymptotically $(k\to\infty)$, to the following relation

$$\frac{a_{k+1}}{a_k}=\frac{2\beta}{k+1}. \tag{18}$$

On the other hand, considering the expansion of the function $e^{2\beta r}$, we obtain

$$e^{2\beta r}=\sum_{k=0}^{\infty}\frac{1}{k!}(2\beta r)^k=1+2\beta r+\cdots+\frac{(2\beta)^k r^k}{k!}+\frac{(2\beta)^{k+1}r^{k+1}}{(k+1)!}+\cdots=\sum_{k=0}^{\infty}b_k r^k.$$

Imposing the asymptotic behaviour $(k\rightarrow\infty)$ in this equation, the b_k − coefficients satisfy

$$\frac{b_{k+1}}{b_k}=\frac{2\beta}{(k+1)}. \tag{19}$$

Comparing Eqs. (18) and (19), one can see that for $k\rightarrow\infty$, the function given by Eq. (16) has the same behaviour than the exponential function $e^{2\beta r}$. As a result, Eq. (16) is converging and then must stop to the term of nth degree, namely

$$a_{k+1}=0 \qquad \text{for } k=n.$$

Thus, according to Eq. (17): $\beta=q/2n$. That means

$$\beta=\frac{Zme^2}{\hbar^2 n}=\frac{Z}{nr_0}, \tag{20}$$

where $r_0=Zme^2/\hbar^2$ denotes the Bohr's radius.

Besides, by use of the solution given by Eq. (17) and the value $k=n$, Eq. (16) is written in the form of a sum of finites terms, namely ($k-l-1=v=0$; $k_{max}-l-1=n-l-1=v$)

$$u(r)=\sum_{k=l+1}^{n}a_k r^k=f^{l+1}\sum_{v=0}^{v=n-l-1}a_{v+l+1}r^v. \tag{21}$$

Using this result, the radial wave function given by Eq. (14) takes the form

$$R(r)=r^l e^{-\beta r}\sum_{v=0}^{v=n-l-1}a_{v+l+1}r^v. \tag{22}$$

We deduce the expression of the incomplete hydrogenic wave function $R(r_1,r_2)$ as follows

$$R_{nl}(r_1,r_2)=r_1^l e^{-\beta^* r_1}\sum_{v=0}^{v=n-l-1}a_{v+l+1}r_1^v\times r_2^l e^{-\beta^* r_2}\sum_{v=0}^{v=n-l-1}a_{v+l+1}r_2^v.$$

That means

$$R_{nl}(r_1,r_2)=(r_1r_2)^l e^{-\beta^*(r_1+r_2)}\sum_{v=0}^{v=n-l-1}a_{v+l+1}(r_1r_2)^v, \tag{23}$$

where

$$\beta^*=\frac{Z^*}{nr_0}=\frac{Z}{n\alpha r_0}. \tag{24}$$

In Eq. (23), the β^*-parameter is the equivalence of the λ-parameter as defined in the Hylleraas wave function. The incomplete hydrogenic wave function is then in the form

$$R_{nl}(r_1,r_2)=(r_1r_2)^l e^{-\frac{Z^*}{nr_0}(r_1+r_2)}\sum_{\nu=0}^{n-l-1} a_{\nu+l+1}(r_1r_2)^\nu. \tag{25}$$

Using this wave function, we determine the expressions of the radial hydrogenic wave functions $R_{10}(r_1,r_2)$, $R_{30}(r_1,r_2)$, $R_{21}(r_1,r_2)$ and $R_{31}(r_1,r_2)$ in Eq. (10) in terms of the coefficient $a_{\nu+l+1}$. We find respectively

$$\text{For } 1s \text{ state}, R_{10}(r_1,r_2)=a_1 e^{-\frac{Z^*}{r_0}(r_1+r_2)}, \tag{26a}$$

$$\text{For } 2s \text{ state}, R_{20}(r_1,r_2)=(a_1+a_2r_1r_2)e^{-\frac{Z^*}{2r_0}(r_1+r_2)}, \tag{26b}$$

$$\text{For } 3s \text{ state}, R_{30}(r_1,r_2)=\left(a_1+a_2r_1r_2+a_3r_1^2r_2^2\right)e^{-\frac{Z^*}{3r_0}(r_1+r_2)}, \tag{26c}$$

$$\text{For } 2p \text{ state}, R_{21}(r_1,r_2)=a_2r_1r_2 e^{-\frac{Z^*}{3r_0}(r_1+r_2)}, \tag{26d}$$

$$\text{For } 3p \text{ state}, R_{31}(r_1,r_2)=\left(a_2r_1r_2+a_3r_1^2r_2^2\right)e^{-\frac{Z^*}{3r_0}(r_1+r_2)}. \tag{26e}$$

Comparing these expressions to those of Eq. (10), we obtain after identification

$$\begin{cases} a_1=1 \\ a_1+a_2=1+\left(\dfrac{Z^*}{2r_0}\right)^2 \\ a_1+a_2+a_3=1+\left(\dfrac{2Z^*}{3r_0}\right)^2+\left(\dfrac{2Z^{*2}}{27r_0^2}\right)^2 \\ a_2+a_3=\left(\dfrac{Z^*}{r_0}\right)^2+\left(\dfrac{Z^{*2}}{6r_0^2}\right)^2 \end{cases} \Rightarrow \begin{cases} a_1=1 \\ a_2=\left(\dfrac{Z^*}{2r_0}\right)^2 \\ a_2=\left(\dfrac{2Z^*}{3r_0}\right)^2,\ a_3=\left(\dfrac{2Z^{*2}}{27r_0^2}\right)^2 \\ a_2=\left(\dfrac{Z^*}{r_0}\right)^2,\ a_3=\left(\dfrac{Z^{*2}}{6r_0^2}\right)^2. \end{cases} \tag{27}$$

2.2 Special incomplete hydrogenic wave functions for (nl^2) symmetric doubly excited states of helium- like ions

Using the preceding results, one can see that the values of a_2 and a_3 disagree. In order to resolve these contradictions, we introduce special incomplete hydrogenic wave functions as follows:

$$\text{For } 1s \text{ state}, R_{10}(r_1,r_2)=e^{-\frac{Z^*}{r_0}(r_1+r_2)}, \tag{28a}$$

$$\text{For } 2s \text{ state}, R_{20}(r_1,r_2)=\left(1+(\rho Z^*)^2r_1r_2\right)e^{-\frac{Z^*}{2r_0}(r_1+r_2)}, \tag{28b}$$

$$\text{For } 3s \text{ state}, R_{30}(r_1,r_2)=\left(1+(\rho Z^*)^2r_1r_2+(\rho Z^*)^4r_1^2r_2^2\right)e^{-\frac{Z^*}{3r_0}(r_1+r_2)}, \tag{28c}$$

$$\text{For } 3p \text{ state}, R_{31}(r_1,r_2)=\left((\rho Z^*)^2r_1r_2+(\rho Z^*)^4r_1^2r_2^2\right)e^{-\frac{Z^*}{3r_0}(r_1+r_2)}. \tag{28d}$$

We obtain as previously

$$\begin{cases} a_1=1 \\ a_1+a_2=1+(\rho Z^*)^2 \\ a_1+a_2+a_3=1+(\rho Z^*)^2+(\rho Z^*)^4 \\ a_2+a_3=(\rho Z^*)^2+(\rho Z^*)^4 \end{cases} \Rightarrow \begin{cases} a_1=1,\ n=1;\ l=0;\ v=0 \\ a_2=(\rho Z^*)^2,\ n=2;\ l=0;\ v=1 \\ a_3=(\rho Z^*)^4,\ n=3;\ l=0;\ v=2 \\ a_2=(\rho Z^*)^2,\ n=2;\ l=1;\ v=1 \\ a_3=(\rho Z^*)^4,\ n=2;\ l=1;\ v=1. \end{cases} \tag{29}$$

In Eq. (29), ρ is a parameter depending on the form of the specific constructed wave function. The coefficients a_{v+l+1} in these equations satisfy the general expression

$$a_{v+l+1}=\Big((\rho Z^*)^2\Big)^{v+l}. \tag{30}$$

By use of this result, we obtain for the radial wave function given by Eq. (25)

$$R_{nl}(r_1r_2)=(r_1r_2)^l e^{-\frac{Z^*}{nr_0}(r_1+r_2)}\sum_{v=0}^{n-l-1}\Big((\varrho Z^*)^2\Big)^{(v+l)}(r_1r_2)^v.$$

This equation can be written in the form

$$R_{nl}(r_1,r_2)=(r_1r_2)^l e^{-\frac{Z^*}{nr_0}(r_1+r_2)}\sum_{v=0}^{n-l-1}(\rho Z^*)^{2v}\times(\rho Z^*)^{2l}\times(r_1r_2)^v,$$

which gives

$$R_{nl}(r_1,r_2)=(r_1r_2)^l e^{-\frac{Z^*}{nr_0}(r_1+r_2)}\sum_{v=0}^{n-l-1}\Big((\rho Z^*)^2(r_1r_2)\Big)^v(\rho Z^*)^{2l}. \tag{31}$$

On the other hand, according to Eqs. (5) and (20)

$$\beta^*=\frac{Z^*}{nr_0}=\frac{Z}{n\alpha r_0}=\lambda.$$

Consequently, $Z^*=nr_0\lambda$. Using these equalities, the special incomplete hydrogenic wave functions given by Eq. (31) can be written in the form

$$R_{nl}(r_1,r_2)=(r_1r_2)^l e^{-\lambda(r_1+r_2)}\sum_{v=0}^{n-l-1}\Big((\rho nr_0\lambda)^2(r_1r_2)\Big)^v(\rho nr_0\lambda)^{2l},$$

which yields

$$R_{nl}(r_1,r_2)=(\rho nr_0\lambda)^{2l}(r_1r_2)^l e^{-\lambda(r_1+r_2)}\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2r_1r_2)^v. \tag{32}$$

Using Eqs. (1), (4) and (32), general special form of Hylleraas correlated waves functions given by Eq. (2) for the description of (nl^2)-symmetric doubly excited state of the helium-like ions are given by

$$\psi_{nl}^{jkm}(r_1,r_2)=(\rho n r_0\lambda)^{2l}(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{_2}|^m e^{-\lambda(r_1+r_2)}.$$

The construction of the special form of Hylleraas correlated waves functions adapted to the correct description of (nl^2) -doubly excited state of helium-like ions becomes very easy by enlightening in the framework of an iterative procedure, the acceptable expression of the ρ-parameter. On the other hand, as the factor $(\rho n r_0\lambda)^{2l}$ will disappear in the calculation of the matrix elements N_{JKM}, $T_{jkmj'k'm'}$, C_{JKM} and W_{JKM}, the above waves functions can be written in the approached form

$$\psi_{nl}^{jkm}(r_1,r_2)=(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}. \tag{33}$$

Let us put $l=n-1$. This involves $n-l-1=0$. We find then the special form of Hylleraas correlated wave functions adapted to the correct description of $2p^2$, $3d^2$ and $4f^2$ symmetric doubly excited state of helium-like ions as follows

$$\psi_{jkmn}(r_1,r_2)=(r_1r_2)^{n-1}(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.$$

These basis wave functions describe the same states than those used by Biaye and co-workers [18]

$$\psi_{jkmn}(r_1,r_2)=(2r_12r_2)^{n-1}(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)},$$

as the 4^{n-1}-coefficient disappears in the calculation of the matrix elements N_{JKM}, $T_{jkmj'k'm'}$, C_{JKM} and W_{JKM}.

In the same way, putting $\rho=2$ in Eq. (33), we get

$$\Psi_{jkmnl}(\vec{r_1},\vec{r_2})=(r_1r_2)^l\sum_{v=0}^{n-l-1}(n^2r_0^2\lambda^22r_12r_2)^v(r_1+r_2)^j(r_1-r_2)^k|r^1\vec{-}\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.$$

Theses wave functions describe again the same states that those used by Biaye and co-workers [19]

$$\Psi_{jkmnl}(\vec{r_1},\vec{r_2})=(2r_12r_2)^l\sum_{v=0}^{n-l-1}(n^2r_0^2\lambda^22r_12r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)},$$

where, the coefficient of proportionality is equal to 4^l and will again disappear when calculating the matrix elements N_{JKM}, $T_{jkmj'k'm'}$, C_{JKM} and W_{JKM}.

2.3 Adequacy of special incomplete hydrogenic wave functions for singlet and triplet doubly excited states of the helium-like ions

Let us here take into account the symmetrization postulate for the correct description of the states of identical particle systems. This will confirm the fact that, general wave functions given by Eq. (33) are suitable as well as for singlet than for triplet excited states of the helium-like ions. According to the symmetrization postulate [24], when a system of particles contains several identical particles, only certain wave functions can describe the physical states of the system. In relation to the nature of the identical particles, these wave functions are either completely symmetric (*for bosons particles*) either completely antisymmetric (*for fermions particles*) with respect to the permutation of the coordinates of the particles. As electrons are fermions, the symmetrization postulate involves that, only are realized the states describe by symmetric $\Psi_s(r_1,r_2)$ and antisymmetric $\Psi_a(r_1,r_2)$ wave functions, namely

$$\Psi_s(r_1,r_2)=\psi_{nl}^{jkm}(r_1,r_2)+\psi_{nl}^{jkm}(r_2,r_1),$$
$$\Psi_a(r_1,r_2)=\psi_{nl}^{jkm}(r_1,r_2)-\psi_{nl}^{jkm}(r_2,r_1).$$

In this expression, the wave functions are symmetric (antisymmetric) under the exchange of the particles 1 and 2 when the plus (minus) sign is used. Considering Eq. (33), we obtain

$$\begin{aligned}\Psi_{jkmnl}(r_1,r_2)=(r_1r_2)^l\sum_{v=0}^{n-l-1}(\varrho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}\\ \pm(r_2r_1)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_2r_1)^v(r_2+r_1)^j(r_2-r_1)^k|\vec{r_2}-\vec{r_1}|^m e^{-\lambda(r_2+r_1)}\end{aligned}$$

As $r_1r_2=r_2r_1$; $(r_1+r_2)=(r_2+r_1)$ and $(r_{12}=|\vec{r_1}-\vec{r_2}|=r_{21}=|\vec{r_2}-\vec{r_1}|)$, the global correlated wave function $\Psi_{jkmnl}(r_1,r_2)$ can be written as follows

$$\begin{aligned}\Psi_{jkmnl}(r_1,r_2)=(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j|\vec{r_1}-\vec{r_2}|^m\\ \times e^{-\lambda(r_1+r_2)}\Big((r_1-r_2)^k\pm(r_2-r_1)^k\Big).\end{aligned}\tag{34}$$

From this expression, one can see that

- if k is even, the antisymmetric wave function is equal to zero and Eq. (34) gives

$$\Psi_{jkmnl}(r_1,r_2)=2(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)};$$

- if k is odd, the symmetric wave function is equal to zero and Eq. (34) gives

$$\Psi_{jkmnl}(r_1,r_2)=2(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.$$

In fact, if k is odd, we can put $k=2q+1$. So

$$(r_2-r_1)^k=(r_2-r_1)^{2q+1}=(r_2-r_1)^{2q}(r_2-r_1)=-(r_1-r_2)^{2q}(r_1-r_2)=-(r_1-r_2)^{2q+1}.$$

That means $(r_2-r_1)^k=-(r_1-r_2)^k$. Inserting this result into Eq. (34), we obtain the last expression of $\Psi_{jkmnl}(r_1,r_2)$.

The preceding results indicate that, the global wave function $\Psi_{jkmnl}(r_1,r_2)$ can be written in the following form

$$\Psi_{jkmnl}(r_1,r_2)=(r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.$$

This special type of trial wave functions constructed by combining Hylleraas and incomplete hydrogenic wave functions [exactly equals to Eq. (33)] is then adapted to the description of both singlet and triplet symmetric doubly excited states of helium isoelectronic series:

- For ^1L singlet doubly excited states, the total spin $S=0$ and the spin wave function is antisymmetric. Subsequently, the spatial wave function is symmetric and we take even values of k -parameter $(k=0,2,4,\cdots)$;

- For ^3L triplet doubly excited states, the total spin $S=1$ and the spin wave function is symmetric. Subsequently, the spatial wave function is antisymmetric and we take odd values of k -parameter $(k=1,3,5,\cdots)$.

On the other hand, for $(nlnl')^{2S+1}L$ doubly excited states, the wave functions are constructed as follows

$$\Psi_{nlnl'}(r_1,r_2)=\psi_{nl}^{jkm}(r_1,r_2)+\psi_{nl'}^{jkm}(r_1,r_2).$$

Using equation Eq. (33), we obtain

$$\begin{aligned}\Psi_{nlnl'}^{jkm}(r_1,r_2)=&\left((r_1r_2)^l\sum_{v=0}^{n-l-1}(\rho^2n^2r_0^2\lambda^2r_1r_2)^v+(r_1r_2)^{l'}\sum_{v=0}^{n-l-1}(\rho^2n'^2r_0^2\lambda^2r_1r_2)^{v'}\right)\\&\times(r_1+r_2)^j(r_1-r_2)^k|\vec{r_1}-\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.\end{aligned}\tag{35}$$

Eq. (35) contains the following wave functions used by Biaye and co-workers [20, 21, 31]

$$\begin{aligned}\Psi_{nlnl'}^{jkm}(r_1,r_2)=&\left((2r_12r_2)^l\sum_{v=0}^{n-l-1}(n^2r_0^2\lambda^22r_12r_2)^v+(r_1r_2)^{l'}\sum_{v=0}^{n-l-1}(n'^2r_0^2\lambda^22r_12r_2)^{v'}\right)\\&\times(r_1+r_2)^j(r_1-r_2)^k|r_1\vec{-}\vec{r_2}|^m e^{-\lambda(r_1+r_2)}.\end{aligned}$$

These wave functions describe the same physical states than Eq. (35) if one takes $\rho=2$.

3 Calculations of energy resonances for $^1P^o$, $^1D^e$, $^1F^o$, $^1G^e$ and $^1H^o$ doubly excited states of He-like ions below the $n = 2 \sim 4$ hydrogenic thresholds

In this section, we apply the screening constant by unit nuclear charge formalism (SCUNC) to calculate the energy resonances of the helium-isoelectronic sequence converging to the $n = 2 \sim 4$ hydrogenic thresholds. In the framework of the SCUNC -method, total energy of $(Nl,nl')^{2S+1}L^{\pi}$ excited states is expressed in the form (in Ryd) [16,17]

$$E(Nlnl',{}^{2S+1}L^{\pi}) = -Z^2\left(\frac{1}{N^2}+\frac{1}{n^2}\left(1-\beta(Nlnl',{}^{2S+1}L^{\pi},Z)\right)^2\right). \tag{36}$$

In this equation, the principal quantum numbers N and n, are respectively for the inner and the outer electron of He-isoelectronic series, the β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by [16,17]

$$\beta(Nlnl',{}^{2S+1}L^{\pi},Z) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k, \tag{37}$$

where $f_k = f_k(Nlnl',{}^{2S+1}L^{\pi})$ are screening constants to be evaluated empirically or variationally.

For $nlnl'^1L^{\pi}$ doubly excited states in two electron systems, the wave functions used in the present calculations is the following using Eq. (35) with $\rho = 1$

$$\Psi_{jkmnll'}(v,w,u) = \left((v^2-w^2)^l \sum_{\mu=0}^{n-l-1}\left(n^2\lambda^2(v^2-w^2)\right)^{\mu} + (v^2-w^2)^{l'}\sum_{\mu'=0}^{n-l'-1}\left(n^2\lambda^2(v^2-w^2)\right)^{\mu'}\right)$$
$$\times v^j w^k\left((v+w)^2+(v-w)^2-u(v^2-w^2)/2\right)^{m/2} e^{-\lambda v}. \tag{38}$$

In this correlated wave function, the λ-parameter is equal to $\lambda = Z/n\alpha$ and the changes $v = (r_1+r_2)$; $w = (r_1-r_2)$; $u = \cos\theta_{12}$ are made. Then for the final wave functions, solution of the Schrödinger's equation, we get

$$\Phi_{n'l'}(\mu,w,u) = \sum_{jkm} a_{jkm}\Psi_{jkmnll'},$$

where the coefficients a_{jkm} are given by solving the following Schrödinger's eigen equation

$$H\Phi_{nll'}(\mu,w,u) = E\Phi_{nll'}(\mu,w,u).$$

In this equation, we remain that the Hamiltonian operator is equal to

$$H = T + C + W,$$

with (in atomic units)

$$T=-\frac{1}{2}(\Delta_1+\Delta_2),\quad C=-\frac{Z}{r_1}-\frac{Z}{r_2},\quad W=\frac{1}{r_{12}}=\frac{1}{|\vec{r_1}-\vec{r_2}|}.$$

Besides, for the representation of the Schrödinger's equation on the non-orthogonal basis, we obtain denoting by q the Hylleraas parameters (j,k,m)

$$\sum_{q'}(H_{nlqq'}-EN_{nlqq'})a_{q'}=0.$$

In this equation, $H_{nlqq'}$ and $N_{nlqq'}$ denote respectively the normalization constant and the matrix elements of the Hamiltonian operator given by

$$H_{nlqq'}=\langle\Psi_{nll'q}|H|\Psi_{nll'q'}\rangle,\qquad N_{nlqq'}=\langle\Psi_{nll'q}|\Psi_{nll'q'}\rangle.$$

Furthermore, in the framework of the screening constant by unit nuclear charge formalism, the β-screening constant is expressed in terms of the variational λ-parameter as follows

$$\beta(nlnl',{}^1L^\pi,Z,\lambda)=\frac{\lambda}{Z^2}\left(1+\frac{l+l'+1}{n+l+l'}\right).$$

As $\lambda=Z/n\alpha$, this equation becomes

$$\beta(nlnl',{}^1L^\pi,Z,\alpha)=\frac{1}{Zn\alpha}\left(1+\frac{l+l'+1}{n+l+l'}\right).$$

Using Eq. (36), total energy of $nlnl'^1L^\pi$ doubly excited states in the helium-like ions is then expressed as follows

$$E(nlnl',{}^1L^\pi)=-\frac{Z^2}{n^2}\left(1+\left(1-\frac{\lambda}{Z^2}\left(1+\frac{l+l'+1}{n+l+l'}\right)\right)^2\right). \tag{39}$$

In this equation, only the λ-parameter is unknown.

The λ-parameter in Eq. (39) is determined by increasing the value of the dimension D of the basis functions until the minima of the functions $(d\langle H(\lambda)\rangle/d\lambda=0)$ converge by exhibiting a plateau according to the Hylleraas and Undheim theorem [22]. The dimension D is given by the (j,k,m)-parameters with the condition $(j,k,m\geq 0)$ and $j+k+m\leq 3$. If λ_0 denotes the value of the λ-parameter corresponding to the minima of the function, a good approximation of the energy positions of $nlnl'^1L^\pi$ doubly excited states in two electron systems is given by

$$E(nlnl',{}^1L^\pi,\lambda_0)=-\frac{Z^2}{n^2}\left(1+\left(1-\frac{\lambda_0}{Z^2}\left(1+\frac{l+l'+1}{n+l+l'}\right)\right)^2\right). \tag{40}$$

4 Results and discussion

The present calculations are carried out in 3×3, 6×6, 10×10 and 13×13 basis corresponding respectively to the dimension of the basis functions $D=3$, 6, 10 and 13. The exhibition of a plateau by the average value $E(\lambda)=\langle H(\lambda)\rangle$ of the Hamiltonian operator arise when $D\geq 10$ and a stabilization is obtained for $D=13$. Then, for the dimension $D=13$ of the basis functions, we compute the values of λ_0 and deduce the $E(nlnl',{}^1L^\pi,\lambda_0)$ energy positions using Eq. (40). The results obtained are listed in Table 1. In Tables 2-4, the comparison of the present calculations up to $Z=10$ with various theoretical calculations and experiments is made.

Table 1: Results for λ_0 and $E(nlnl',{}^1L^\pi,\lambda_0)$ energy positions of the helium-like ions up to Z=10. All results are expressed in atomic units.

	Z	2	3	4	5	6	7	8	9	10
$2s2p\,{}^1P^o$	λ_0	0.8324	1.5158	1.7579	2.2390	2.7125	3.1952	3.6517	4.1081	4.6091
	$-E$	0.7133	1.70701	3.3346	5.3867	7.9407	10.9910	14.5508	18.6106	23.1533
$3s3p\,{}^1P^o$	λ_0	0.7199	1.1718	1.5088	1.9088	2.2906	2.7052	3.0916	3.5213	3.9125
	$-E$	0.3406	0.8238	1.5441	2.4779	3.6364	5.0122	6.6145	8.4322	10.4782
$4s4p\,{}^1P^o$	λ_0	0.8590	1.2324	1.5748	1.9685	2.3622	2.6457	3.0236	3.4016	3.7795
	$-E$	0.1861	0.4650	0.8717	1.3997	2.0528	2.8397	3.7442	4.7736	5.9280
$3s3d\,{}^1D^e$	λ_0	0.7544	1.1453	1.5271	1.9562	2.3475	2.7732	3.1694	3.5656	4.0122
	$-E$	0.3306	0.8171	1.5270	2.4518	3.6044	4.9737	6.5699	8.3884	10.4207
$4s4d\,{}^1D^e$	λ_0	0.8590	1.2324	1.5748	1.9685	2.3622	2.6457	3.0236	3.4016	3.7795
	$-E$	0.1824	0.4588	0.8633	1.3888	2.0394	2.8245	3.7266	4.7536	5.9057
$4s4f\,{}^1F^o$	λ_0	0.8999	1.3498	1.7180	2.1474	2.4649	2.8757	3.1496	3.5433	3.9370
	$-E$	0.1772	0.4455	0.8455	1.3658	2.0209	2.7931	3.7026	4.7265	5.8753
$3p3d\,{}^1F^o$	λ_0	0.9332	1.3793	1.8127	2.2337	2.6804	3.1272	3.5739	4.0207	4.4675
	$-E$	0.3052	0.7772	1.4738	2.3949	3.5344	4.8961	6.4801	8.2862	10.3146
$4p4d\,{}^1F^o$	λ_0	0.8590	1.2324	1.5748	1.9685	2.3622	2.6457	3.0236	3.4016	3.7795
	$-E$	0.1799	0.4545	0.8573	1.3811	2.0299	2.8137	3.7141	4.7394	5.8898
$4p4f\,{}^1G^e$	λ_0	0.8999	1.3498	1.7180	2.1474	2.4649	2.8757	3.1496	3.5433	3.9370
	$-E$	0.1753	0.4421	0.8407	1.3596	2.0136	2.7844	3.6929	4.7154	5.8629
$4d4f\,{}^1H^o$	λ_0	0.8999	1.3498	1.7180	2.1474	2.4649	2.8757	3.1496	3.5433	3.9370
	$-E$	0.1738	0.4395	0.8370	1.3548	2.0079	2.7776	3.6854	4.7069	5.8533

Considering the results listed in Table 2 for $2s2p\,{}^1P^o$, $3s3p\,{}^1P^o$, $4s4p\,{}^1P^o$ and $3s3d\,{}^1D^e$ levels, the agreement between the present calculations and the double sums over the complete hydrogen spectrum values of Ivanov and Safronova [8], the complex rotation results of Ho [9, 10], the Feshbach projection results of Bachau *et al.* [14] and with our semi-empirical results obtained previously [16, 17] is seen to be good. One can also remark that, the present variational results are close to that of the complex rotation calculations [9] for $2s2p\,{}^1P^o$ levels for $Z=3\sim9$. For $3s3p\,^1P^o$ level, the agreement between the present calculations and the semi-empirical results we obtain previously [16] is seen to be very good. Comparison between the two procedures (variational and semi-empirical) of the SCUNC-method for the $2s2p\,^1P^o$ and $4s4p\,^1P^o$ levels shows an agreement that can be considered to be very satisfactory.

Table 2: Comparison of $E(nlnl'\,^1L^\pi)$ energy positions of the helium-like ions up to Z=10 between the present calculations and various other results. All results are expressed in atomic units.

	Z	2	3	4	5	6	7	8	9	10
$2s2p\,^1P^o$	$-E^p$	0.7133	1.7070	3.3346	5.3867	7.9407	10.9910	14.5508	18.6106	23.1533
	$-E^a$	0.6944	1.7556	3.3179	5.3779	7.9414	11.0031	14.5649	18.6266	23.1884
	$-E^b$	0.6931	1.7576	3.3195	5.3802	7.9403	10.9999	14.5594	18.6187	23.1778
	$-E^c$	0.7137	1.7723	3.3309	5.3895	7.9481	11.0067	14.5653	18.6239	23.1825
	$-E^d$	0.7136	1.7747	3.3684	5.4276	7.9815	11.0960	14.6733	18.7326	23.2633
$3s3p\,^1P^o$	$-E^p$	0.3406	0.8238	1.5441	2.4779	3.6364	5.0122	6.6145	8.4322	10.4782
	$-E^e$	0.3344	0.8257	1.5391	2.4747	3.6327	5.0126	6.6152	8.4398	10.4864
	$-E^f$	0.3356	0.8288	1.5438	2.4809	3.6402	5.0217	6.6255	8.4514	10.4995
	$-E^c$	0.3044	0.7771	1.4719	2.3891	3.5284	4.8899	6.4737	8.2797	10.3079
	$-E^d$	0.3313	0.8369	1.5771	2.5523	3.7630	5.2093	6.8913	8.8089	10.9625
$4s4p\,^1P^o$	$-E^p$	0.1861	0.4650	0.8717	1.3997	2.0528	2.8397	3.7442	4.7736	5.9280
	$-E^e$	0.1966	1.4788	0.8856	1.4178	2.0749	2.8572	3.7642	4.7635	5.9534
	$-E^b$	0.1944	0.4759	0.8823	1.4134	2.0693	2.8503	3.7642	4.7873	5.9431
	$-E^d$	0.1798	0.4497	0.8431	1.3607	2.0028	2.7697	3.6616	4.6786	5.8207
$3s3d\,^1D^e$	$-E^p$	0.3306	0.8171	1.5270	2.4518	3.6044	4.9737	6.5699	8.3884	10.4207
	$-E^g$	0.3149	0.7957	1.4980	2.4230	3.5700	4.9380	6.5300	8.3430	10.3800
	$-E^c$	0.3184	0.7962	1.4963	2.4186	3.5632	4.9299	6.5189	8.3301	10.3635
	$-E^d$	0.3232	0.8149	1.5347	2.4834	3.6612	5.0683	6.7049	8.5343	10.5932

^{p} present work, variational calculations.
^{a} Sakho *et al.* [17], semi-empirical calculations.
^{b} Ho [8], complex rotation method.
^{c} Ivanov and Safronova [8], double sum method over the complete hydrogen spectrum.
^{d} Biaye *et al.* [20], variational calculations.
^{e} Sakho *et al.* [16], semi-empirical calculations.
^{f} Ho [10], complex rotation method.
^{g} Bachau *et al.* [14], Feshbach projection method.

In Table 3, the results obtained for $4s4d\,^1D^e$, $4s4f\,^1F^o$, $3p3pd\,^1F^o$, $4p4d\,^1F^o$, $4p4f\,^1G^e$ and $4d4f\,^1H^o$ resonances in the helium-like ions up to $Z=10$ are displayed and compared with the double sums over the complete hydrogen spectrum results of Ivanov and Safronova [8], the complex rotation values of Ho and Bhatia [11] and of Bhatia and Ho [12], the density functional theory of Roy *et al.* [13] and with the Feshbach-projection results of Bachau *et al.* [14]. It can be seen that, the present calculations agree well with those of the cited authors. It appears that the results obtain for $3p3d\,^1F^o$ and $4p4d\,^1F^o$ levels match well with the complex rotation results of Ho and Bhatia [11] and with that of Bhatia and Ho [12]

Table 3: Comparison of $E(nlnl'^1L^\pi)$ energy positions of the helium-like ions up to Z=10 between the present calculations and various other results. All results are expressed in atomic units.

	Z	2	3	4	5	6	7	8	9	10
$4s4d\,^1D^e$	$-E^p$	0.1824	0.4588	0.8633	1.388	2.0394	2.8245	3.7266	4.7536	5.9057
	$-E^a$		0.4639	0.8652	1.3913	2.0425	2.8186	3.7204	4.7463	5.8972
	$-E^b$	0.1798	0.4497	0.8431	1.3606	2.0027	2.7697	3.6615	4.6785	5.8206
$3p3d\,^1F^o$	$-E^p$	0.3052	0.7772	1.4738	2.3949	3.5344	4.8961	6.4801	8.2862	10.3146
	$-E^c$	0.3041	0.7710	1.4580	2.3660	0.4960	4.8480	6.4220	8.2190	10.2400
	$-E^d$	0.3044	0.7671	1.4519	2.3589	3.4882	4.8396	6.4133	8.2093	10.2774
	$-E^b$	0.3168	0.7960	1.4969	2.4205	3.5674	4.9377	6.5317	8.3433	10.3907
	$-E^e$	0.2782	0.7445	1.4328	2.3433					
$4s4f\,^1F^o$	$-E^p$	0.1772	0.4455	0.8455	1.3658	2.0209	2.7931	3.7026	4.7265	5.8753
	$-E^f$		0.4508	0.8470	1.3678	2.0135	2.7842	3.6798	4.7004	5.8460
	$-E^b$	0.1797	0.4493	0.8422	1.3591	2.0003	2.7661	3.6567	4.6721	5.8124
$4p4d\,^1F^o$	$-E^p$	0.1799	0.4545	0.8573	1.3811	2.0299	2.8137	3.7141	4.7394	5.8898
	$-E^f$		0.4641	0.8650	1.3910	2.0421	2.8182	3.7194	4.7455	5.8967
	$-E^b$	0.1798	0.4497	0.8431	1.3606	2.0027	2.7697	3.6615	4.6785	5.8206
	$-E^e$	0.1593	0.4233	0.8123	1.3262					
$4p4f\,^1G^e$	$-E^p$	0.1753	0.4421	0.8407	1.3596	2.0136	2.7844	3.6919	4.7154	5.8629
	$-E^b$	0.1797	0.4493	0.8422	1.3591	2.0003	2.7661	3.6567	4.6721	5.8124
$4d4f\,^1H^o$	$-E^p$	0.1738	0.4395	0.8370	1.3548	2.0079	2.777	3.6854	4.7069	5.8533

[p] present work.
[a] Ho and Bhatia [11], complex rotation method.
[b] Biaye *et al.* [20], variational calculations.
[c] Bachau *et al.* [14], Feshbach projection method.
[d] Ivanov and Safronova [8], double sum method over the complete hydrogen spectrum.
[e] Roy *et al.* [13], density functional theory.
[f] Bhatia and Ho [12], complex rotation method.

for $Z = 3 \sim 10$. As far as comparison with the variational calculations of Biaye *et al.* [20] is concerned, the agreement is seen to be satisfactory. Let us underline that, the results of Biaye *et al.* [20] have been obtained using Eq. (35) where $\rho = 2$ and by applying the Hylleraas and Undheim theorem [30]. The eigenvalues are obtained when the minima of the functions converge with increasing the values of the dimension D of the states. It is seen that, discrepancies appear when the charge number Z increases. Biaye *et al.* [19,20] explain these slight disagreement for higher Z by the choice of the angular part of the wave functions which describe better the atomic system with low-Z than with high-Z and by the fact that they have also omitted the Feshbach shifts in their calculations. But, it should be mentioned that, when we combine the Hylleraas variational principal to the SCUND method, the results obtained by using the wave functions given Eq. (35) with $\rho = 1$, are more accurate. This is demonstrated by comparing the results quoted as well as in Table 2 for $2s2p\,^1P^o$, $3s3p\,^1P^o$ and $4s4p\,^1P^o$ levels than in Table 3 for $4s4p\,^1D^e$, $4s4f\,^1F^o$, $3p3d\,^1F^o$, $4p4d\,^1G^e$ and $4d4f\,^1H^o$ resonances.

Table 4: Comparison of the present $E(nlnl'\,^1L^\pi)$ energy positions of the helium-like ions up to Z=10 with experiments and other calculations. The excitation energies are calculated with respect to the ground state of the corresponding systems and the infinite rydbergs (13.605698 eV) is used for energy conversion. All results are expressed in eV: 1 a.u = 2 Ryd. The accurate ground state energies of Frankowsky and Pekeris [30] are used in the present calculations respectively (in atomic units): 2.90372 (He) 7.27991 (Li^+); 13.65556 (Be^{2+}) and 22.03097 (B^{3+}).

	Z	2	3	4	5
$2s2p\,^1P^o$	$-E^p$	59.60	151.65	280.85	452.91
	$-E^a$	60.13	150.34	281.35	456.15
	$-E^{b,c}$	60.13^b	150.31^c		
$3s3p\,^1P^o$	$-E^p$	69.75	175.68	329.57	532.07
	$-E^a$	69.91	175.63	330.54	532.15
	$-E^b$	69.91			
$4s4p\,^1P^o$	$-E^p$	73.95	185.44	347.87	561.41
	$-E^a$	73.66	185.07	347.49	560.91
	$-E^d$	73.66			
$3p3d\,^1F^o$	$-E^p$	70.71	176.95	331.48	534.32
	$-E^e$	71.44	177.84	332.59	535.73
	$-E^g$	70.52	176.90	331.98	535.05
$4p4d\,^1F^o$	$-E^p$	74.12	185.73	348.26	561.91
	$-E^e$	74.68	186.58	349.48	563.40
	$-E^f$	73.95	185.89	348.72	562.55

[p] present work, variational calculations.

[a] Sakho *et al.* [16], semi-empirical calculations.

[b] Experiment, Kossman *et al.* [26]

[c] Experiment, Diehl *et al.* [27].

[d] Experiment, Woodruff and Samson [28].

[e] Roy *et al.* [13].

[f] Ray *el al.* [25].

In Table 4, the comparison of excitation energy of $2s2p\,^1P^o$, $3s3p\,^1P^o$, $4s4p\,^1P^o$, $3s3d\,^1D^e$ and $4p4d\,^1F^o$ levels for $Z=2\sim5$ is made with available experimental and theoretical literature values. For $2s2p\,^1P^o$, $3s3p\,^1P^o$ and $s4p\,^1P^o$ levels, comparison indicates that both variational and semi-empirical procedures of the SCUNC-method give results matching very well. As far as $3s3d\,^1D^e$ and $4p4d\,^1F^o$ levels are concerned, it appears that our results agree as well as with that of Roy *et al.* [13] than with that of Ray *el al.* [25]. As regard comparison with experiments, the agreements between the results obtained in the present work and the experimental data of Kossman *et al.* [26], Diehl *et al.* [27] and of Woodruff and Samson [28] for $2s2p\,^1P^o$, $3s3p\,^1P^o$ and $4s4p\,^1P^o$ levels of He and Li^+ are seen to be very satisfactory.

On the other hand, it is interesting to mention that the semi-empirical procedure of the SCUNC-method is most soft that the variational procedure. In addition, the most important point to underline is that, in the framework of the semi-empirical procedure of the SCUNC-method, it is not necessary to invoke calculations requiring a fair amount of mathematical complexity nor a computer program to succeed in obtaining accurate results in the treatment of the properties of the helium isoelectronic sequence. This is not the case of the variational procedure for the main following reasons. First, one may construct the adequate expression of the correlated wave function to be used in the calculations. Such a task is not easy and it can take many months (that is not the case of the semi-empirical procedure where the establishment of the energy expressions takes less than one week when experimental data are available). Secondly, an adequate computer program (Fortran in the present calculations) is to be concocted for computations and, generally, such program is very fastidious (for the semi-empirical procedure, energies are directly calculated).

In summary, it has been demonstrated in the present work the possibilities to use the screening constant by unit nuclear charge method in the study of $nlnl'$ doubly excited states in the helium-like ions in the framework of a variational procedure. Correlated wave functions combining Hylleraas to incomplete hydrogenic wave functions are used in the present computations and accurate results are obtained as shown by the comparison with various available theoretical and experimental literature values. One can notice that, the merit of the screening constant by unit nuclear charge method is to give the possibilities to calculate accurate energies for doubly excited states in two electron systems using a variational procedure or a semi-empirical one.

Acknowledgments. The author is greatly indebted to Dr. M. Biaye for the computational part of the present work and for helpful discussions. The author also thanks Prof. A. Wagué for his support.

References

[1] G. W. Kellner, Z. Phys. 44 (1927) 91.
[2] E. A. Hylleraas, Z. Phys. 48 (1928) 469.
[3] R. P. Madden and K. Colding, Phys. Rev. Lett. 10 (1963) 516.
[4] K. Codling, R. P. Madden, and D. L. Ederer, Phys. Rev. 155 (1967) A26.
[5] J. W. Cooper, U. Fano, and F. Prats. Phys. Rev. Lett. 10 (1963) 518.
[6] D. R. Herrick and O. Sinanoglu, Phys. Rev. A 11 (1975) 97.
[7] S. M. Kahn, Phys. Scr. T 80 (1999) 23.
[8] A. I. Ivanov and I. U. Safronova, Opt. Spectrosc. 75 (1993) 506.
[9] Y. K. Ho, Phys. Lett. A 79 (1980) 44.
[10] Y. K. Ho, J. Phys. B: At. Mol. Opt. Phys. 12 (1979) 387.
[11] Y. K. Ho and A. K. Bhatia, Phys. Rev. A 44 (1991) 2895.
[12] A. K. Bhatia and Y. K. Ho, J. Phys. B: At. Mol. Opt. Phys. 31 (1998) 3307.
[13] A. K. Roy, R. Singh, and B. M. Debyz, J. Phys. B: At. Mol. Opt. Phys. 30 (1997) 4763.
[14] H. Bachau, F. Martin, A. Riera, and M. Yanez, At. Data Nucl. Data Tab. 48 (1991) 167.
[15] I. Sakho, A. S. Ndao, M. Biaye, and A Wagué, Phys. Scr. 74 (2006) 180.

[16] I. Sakho, A. S. Ndao, M. Biaye, and A Wagué, Eur. Phys. J. D 47 (2008) 37.

[17] I. Sakho, A. Konté, A. S. Ndao, *et al.*, Phys. Scr. 77 (2008) 055303.

[18] M. Biaye, A. Konté, B. A. N. Faye, and A. Wagué, Eur. Phys. J. D 13 (2001) 21.

[19] M. Biaye, A. Konté, B. A. N. Faye, and A. Wagué, Phys. Scr. 71(2005) 39.

[20] M. Biaye, A. Konté, B. A. N. Faye, and A. Wagué, Phys. Scr. 71(2005) 373.

[21] M. Biaye, M. Dieng, I. Sakho, *et al.*, Chinese J. Phys. 47 (2009) 166.

[22] E. A. Hylleraas and B. Undheim, Z. Phys. 65 (1930) 759.

[23] D. Sivoukhine, Cours de Physique Générale Tome V: Physique Atomique et Nucléaire (Mir, Moscou, 1986).

[24] C. Cohen-Tanoundji, D. Bernard, and L. Franck, Mécanique Quantique 2 (Hermann Editeurs des Sciences et des. Arts, Paris, 1992).

[25] D. Ray, M. Sugawara, Y. Fujimura, *et al.*, Phys. Lett. A 169 (1992) 452.

[26] H. Kossman, B. Krassig and V. Schmidt, J. Phys. B: At. Mol. Opt. Phys. 21 (1988) 1489.

[27] S. Diehl, D. Cubaynes, J. M. Bizau, *et al.*, J. Phys. B: At. Mol. Opt. Phys. 32 (1999) 4193.

[28] D. R. Woodruff and J. A. R. Samson, Phys. Rev. Lett. 25 (1982) 848.

[29] Y. K. Ho, Z. Phys. D 21 (1991) 191.

[30] F. Frankowski and C. L. Pekeris, Phys. Rev. 146 (1966) 46.

[31] M. Dieng, I. Sakho, M. Biaye, and A. Wagué, Chinese J. Phys. 48 (2010) 38.