



Review Article

Variationnal Calculation of the Doubly $(nl)^2 \ ^1L^\pi$ Excited States of He-Like Ions Via the Screening Constant by Unit Nuclear Charge Formalism

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Abstract: The present work deals with an *ab initio* calculation of total energies of the doubly excited np^2 , nd^2 and nf^2 states in the helium-like systems. These total energies are calculated in the framework of the variationnal procedure of the Screening constant by unit nuclear charge (SCUNC) formalism. In the present work, a new correlated wave function is presented to express analytically the total energies of the doubly np^2 , nd^2 and nf^2 excited states in the He-like systems. The present results obtained up to $Z = 10$ and $n = 4$ agree very well with various computational methods.

Keywords: *Ab Initio* Calculation, Doubly Excited, Total Energy, Helium-Like Systems, Correlated Wave Function, Screening Constant by Unit Nuclear Charge

1. Introduction

Over the last two decades, various methods have been performed to understand electron-electron correlation effects in doubly (nl^2) excited states of He-like systems. Although many accurate data have been tabulated for these doubly excited states, the methods used require in general, complexity in the variationnal procedure along with the use of computational codes. Subsequently, energy of the doubly (nl^2) excited states of He-like systems cannot be expressed analytically from various *ab initio* methods such as the complex rotation method [1-3], the variationnal method of Hylleraas [4], the double sums over the total hydrogen spectrum formalism [5], the density functional theory [6], the formalism of the Feshbach projection operators [7, 8], the discretization technique [9], the truncated diagonalization method [10], the time-dependent variation perturbation theory

[11], to name a few. In contrast with these *ab initio* methods applied in the analysis of two atomic systems spectra, the Screening constant by unit nuclear charge (SCUNC) formalism has the advantages to provide accurate energy position within a simple semi-empirical procedure as well as for the doubly $(Nlnl' \ ^{2S+1}L)$ [12, 13] excited state than in the mixed configurations based on the classification scheme designated by the notation ${}_N(K,T)_n^{A \ 2S+1} L^\pi$ [14-17]. The variationnal procedure of the SCUNC formalism has been applied successfully only in 2006 for the ground state of He-like ions [18]. From this date, only the semi-empirical procedure of the SCUNC formalism based on experimental data has been used [12-17]. But this semi-empirical procedure requires the use of experimental data as input to evaluate the fitting parameters in the energy expressions. This means that, when experimental data are unavailable, the SCUNC formalism becomes unsuitable. As most of the doubly (nl^2)

excited states in He-like ions no experimental data are available, it becomes very challenging to develop the variational procedure of the SCUNC formalism on these excited states. Then, the goal of the present work is to apply for the first time, the variational procedure of the SCUNC formalism in the calculation of energies of the doubly (nl^2) excited. The present study is focused firstly on the doubly $np^2 \ ^1D^e$, $nd^2 \ ^1G^e$ and $nf^2 \ ^1F^e$ excited states of two-electron atomic systems. After, the formalism can be extended to the study of the excited states of more complex atomic systems. Section 2 gives a brief description of the variational procedure of the SCUNC formalism adopted in this work. The results obtained

are displayed and discussed in section 3. Conclusion of the present study is made in section 4.

2. Theory

2.1. Energy of the Doubly (nl^2) Excited States

In the framework of the Screening constant by unit Nuclear charge formalism, total energies of the doubly (Nl, nl') $^{2S+1}L^\pi$ excited states are expressed in the form

$$E(Nlnl'; \ ^{2S+1}L^\pi) = -Z^2 \left(\frac{1}{N^2} + \frac{1}{n^2} \left[1 - \beta(Nlnl'; \ ^{2S+1}L^\pi; Z) \right]^2 \right) Ryd \quad (1)$$

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

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

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

In the framework of the semi-empirical procedure of the SCUNC formalism, the f_k parameters are evaluated from

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - \frac{f_1(n, l, \ ^1L^\pi; Z)}{Z} - \frac{f_2(n, l, \ ^1L^\pi; Z)}{Z^2} - \frac{f_3(n, l, \ ^1L^\pi; Z)}{Z^3} \right)^2 \right\} \quad (4)$$

To facilitate the calculation of $E(nl)$, the dependence of f_1 with n is neglected and both f_2 and f_3 are expressed in term of f_1 . So, the f_k -parameters ($k=2, 3$) are in the form:

$$f_k(l, Z, \ ^1L^\pi) = \frac{g_k(l, Z)}{h_k(n, l)} \times f_1(l, \ ^1L^\pi, Z). \quad (5)$$

where

$$\begin{cases} g_k(l, Z) = k - 2 + l(Z - 1) \\ h_k(n, l) = (k - 2)[2n - l - (k - 1)] \end{cases} \quad \text{if } l \text{ is odd.} \quad (6)$$

$$\begin{cases} f_2(l, Z, \ ^1L^\pi) = l(Z - 1) \times f_1(l, \ ^1L^\pi, Z) \\ f_3(l, Z, \ ^1L^\pi) = \frac{l(Z - 1) + 1}{(2n - l - 2)} \times f_1(l, \ ^1L^\pi, Z) \end{cases} \quad \text{if } l \text{ is odd.} \quad (8)$$

and

$$\begin{cases} f_2(l, Z, \ ^1L^\pi) = l(Z - 1) \times f_1(l, \ ^1L^\pi, Z) \\ f_3(l, Z, \ ^1L^\pi) = \frac{l(Z - 1) + 1}{(n - l + 1)} \times f_1(l, \ ^1L^\pi, Z) \end{cases} \quad \text{if } l \text{ is even.} \quad (9)$$

experimental data on a given element of Z -atomic number. As a result, the f_k -screening constants depend also on Z as well as on the n - principal quantum number and on the l - orbital quantum number. So, for the doubly $(nl)^2$ ($l \neq 0$) excited states considered in this work, total energies are expressed as follows

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - \sum_{k=1}^q f_k(n, l, \ ^1L^\pi; Z) \times \left(\frac{1}{Z} \right)^k \right)^2 \right\} \quad (3)$$

In the present work, the expansion is limited to $q=3$. So Eq. (3) is written in the form:

and

$$\begin{cases} g_k(l, Z) = k - 2 + l(Z - 1) \\ h_k(n, l) = (k - 2)[n - l + (k - 2)] \end{cases} \quad \text{if } l \text{ is even.} \quad (7)$$

The present study is devoted to the np^2 , nd^2 and nf^2 states. Then Eqs. (6) are for the np^2 , and nf^2 states for which l is odd and respectively equal to 1 and 3. Eqs. (7) are for the nd^2 state as $l = 2$. Using Eqs. (6) and (7), Eq. (5) gives

Total energies can then be expressed as follows

1. For the np^2 ($l = 1$) and nl^2 ($l = 3$) doubly excited states

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - f_1(l, {}^1L^\pi, Z) \frac{1}{Z} - f_1(l, {}^1L^\pi, Z) \frac{l(Z-1)}{Z^2(2n-l-2)} - f_1(l, {}^1L^\pi, Z) \frac{l(Z-1)+1}{Z^3} \right)^2 \right\} \quad (10)$$

2. For the nd^2 ($l = 2$) doubly excited states

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - f_1(l, {}^1L^\pi, Z) \frac{1}{Z} - f_1(l, {}^1L^\pi, Z) \frac{l(Z-1)-1/2}{Z^2(n-l+1)} - f_1(l, {}^1L^\pi, Z) \frac{l(Z-1)+1/2}{Z^3} \right)^2 \right\} \quad (11)$$

In Eqs. (10) and (11), only one fitting parameter e.g. f_1 is unknown. This parameter is easily evaluated from the semi-empirical procedure of the SCUNC formalism using experimental data as demonstrated in more than twenty published papers since 2006. As mentioned in the introduction, for all the previous SCUNC studies [12–17], the variational

procedure of the SCUNC formalism has been applied only in the first paper [18] devoted to the ground state of He-like ions. In addition for the ground state, the total energies of the He-like systems have been expressed variationally as follows (in Rydberg units)

$$E(1s) = -Z^2 \times \left\{ 1 + \left(1 - f_1(s, {}^1S^e, Z) \frac{1}{Z} \right)^2 \right\} = -Z^2 \times \left\{ 1 + \left(1 - \frac{0,625}{Z} \right)^2 \right\} \quad (12)$$

This equation shows that $f_1(s, {}^1S^e, Z) = 0,625$. For the highly charge Si^{14+} ion, Eq. (12) gives $E(1s) = -5100.65$ eV to be compared to the accurate theoretical value obtained by Drake [19] at -5100.58 eV. This indicates that, the dependence of

the $f_1(s, {}^1S^e, Z)$ –screening constant with Z can be neglected with a good approximation. So, for the doubly (nl^2) excited states, using $f_1(s, {}^1S^e, Z) = f_1(l, {}^1L^\pi)$, Eqs. (10) and (11) are rewritten as follows

a) For the np^2 ($l = 1$) and nl^2 ($l = 3$) doubly excited states

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - f_1(l, {}^1L^\pi) \frac{1}{Z} - f_1(l, {}^1L^\pi) \frac{l(Z-1)}{Z^2(2n-l-2)} - f_1(l, {}^1L^\pi) \frac{l(Z-1)+1}{Z^3} \right)^2 \right\} \quad (13)$$

b) For the nd^2 ($l = 2$) doubly excited states

$$E(nl) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - f_1(l, {}^1L^\pi) \frac{1}{Z} - f_1(l, {}^1L^\pi) \frac{l(Z-1)-1/2}{Z^2(n-l+1)} - f_1(l, {}^1L^\pi) \frac{l(Z-1)+1/2}{Z^3} \right)^2 \right\} \quad (14)$$

To evaluated theoretically the $f_1({}^1L^\pi)$ -screening constant in Eqs. (13) and (14), the first step consists of constructing the appropriated correlated wave function for the doubly (nl^2) excited states. After, the $f_1({}^1L^\pi)$ -parameter is determined from the Ritz's variation principle.

2.2. Appropriated Correlated Wave Function for the DES (nl^2) States

To construct the appropriated correlated wave function for the DES (nl^2) states, the starting point is the use of incomplete radial hydrogenic wave functions for the 2p, 3d and 4f states expressed below

1. for a 2p-electron:

$$R_{2,1}(r) = r e^{-\frac{Zr}{2a_0}}, \quad l = 1. \quad (15)$$

2. for a 3d-electron:

$$R_{3,2}(r) = r^2 e^{-\frac{Zr}{3a_0}}, \quad l = 2. \quad (16)$$

3. for a 4f-electron:

$$R_{4,3}(r) = r^3 e^{-\frac{Zr}{4a_0}}, \quad l = 3. \quad (17)$$

The incomplete radial wave functions (15), (16) and (17) can be written in a single expression as follows

$$R_{n,l}(r) = r^l e^{-\frac{Zr}{na_0}} \quad (18)$$

For the helium isoelectronic sequence containing two electrons, r_1 and r_2 being their radial coordinates, Eq. (13) becomes in the framework of the independent particles model

$$R_{n,l}(r_1, r_2) = (r_1 r_2)^l e^{-\frac{Z}{na_0}(r_1+r_2)} \quad (19)$$

Taking into account electron-electron correlation effects occurring in He-like systems, the Z^* - effective charge number is introduced by constructing the correlated wave function as follows:

$$\Psi(r_1, r_2) = (r_1 r_2)^l e^{-\frac{Z^*}{na_0}(r_1+r_2)} \quad (20)$$

where the effective charge number is given by

$$Z^* = Z \times (2l+1) \left(1 - \frac{f_1(l, L^\pi)}{Z} \right). \quad (21)$$

As far as the variational parameter α is concerned, it is given by

$$\alpha_n = \frac{(2l+1)}{n} \times Z \left(1 - \frac{f_1(l, L^\pi)}{Z} \right) \quad (22)$$

In atomic units, $a_0 = 1$. Taking into account Eq. (20), the correlated wave function (18.a) is written in the form:

$$\Psi(r_1, r_2; \alpha_n) = (r_1 r_2)^l e^{-\alpha_n(r_1+r_2)} \quad (23)$$

$$\begin{aligned} N E(\alpha) = & \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 + \left(\frac{\partial \Psi}{\partial t} \right)^2 + \left(\frac{\partial \Psi}{\partial u} \right)^2 \right] + 2 \left(\frac{\partial \Psi}{\partial u} \right) \times \left[s(u^2 - t^2) \frac{\partial \Psi}{\partial s} + \right. \right. \\ & \left. \left. + t(s^2 - u^2) \frac{\partial \Psi}{\partial t} \right] - \Psi^2 [4Zsu - s^2 + t^2] \right\} \end{aligned} \quad (29)$$

As far as the correlated wave function is concerned, it is expressed in the form

$$\Psi(s, t, \alpha_n) = \frac{1}{4} (s^2 - t^2) e^{-\alpha_n s} \quad (30)$$

3. Results and Discussion

Using the correlated wave function (30), Eq. (29) provides (see appendix for details for the particular case of the np^2 levels, the procedure is the same for nd^2 and nf^2)

1. for the np^2 states

$$E(\alpha_2) = \frac{1}{3} \alpha_2^2 - \left(Z - \frac{93}{256} \right) \alpha_2. \quad (31)$$

2. for the nd^2 states

$$E(\alpha_3) = \frac{1}{5} \alpha_3^2 - \left(\frac{2}{3} Z - \frac{793}{3072} \right) \alpha_3. \quad (32)$$

3. for the nf^2 states

In addition, the Hamiltonian of the helium isoelectronic series is given by (in atomic units)

$$H = -\frac{1}{2} \Delta_1 - \frac{1}{2} \Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (24)$$

In the framework of the Ritz' variation principle, the energy $E(\alpha)$ is obtained from the condition

$$\frac{d \langle H \rangle(\alpha)}{d\alpha} \Big|_{\alpha=\alpha(0)} = 0 \quad (25)$$

In Eq. (25), $E(\alpha) = \langle H \rangle(\alpha)$ with

$$E(\alpha) = \langle H \rangle(\alpha) = \frac{\langle \Psi(\alpha) | H | \Psi(\alpha) \rangle}{\langle \Psi(\alpha) | \Psi(\alpha) \rangle} \quad (26)$$

The integration of Eq. (26) is facilitated by turning into account a change of variables using elliptical coordinates [18]

$$s = (r_1 + r_2); \quad t = (r_1 - r_2); \quad u = r_{12}. \quad (27)$$

$$d\tau = d^3 r_1 d^3 r_2 = 2\pi^2 (s^2 - t^2) u ds dt du. \quad (28)$$

Using these elliptical coordinates, Eq. (26) is rewritten as follows

$$E(\alpha_4) = \frac{1}{7} \alpha_4^2 - \left(\frac{1}{2} Z - \frac{26333}{131072} \right) \alpha_4. \quad (33)$$

From the variational principle, one can write

$$\frac{E(\alpha)}{d\alpha} \Big|_{\alpha=\alpha(0)} = 0 \quad (34)$$

So Eqs. (31), (32) and (33) provide respectively

1. for the np^2 states

$$\alpha_2(0) = \frac{3}{2} \left(Z - \frac{93}{256} \right) = \frac{3}{2} Z \left(1 - \frac{93}{256} \times \frac{1}{Z} \right). \quad (35)$$

2. for the nd^2 states

$$\alpha_3(0) = \frac{5}{2} \left(\frac{2}{3} Z - \frac{793}{3072} \right) = \frac{5}{3} Z \left(1 - \frac{2379}{6144} \times \frac{1}{Z} \right). \quad (36)$$

3. for the nf^2 states

$$\alpha_4(0) = \frac{7}{2} \left(\frac{1}{2} Z - \frac{26333}{131072} \right) = \frac{7}{4} Z \left(1 - \frac{26333}{65536} \times \frac{1}{Z} \right). \quad (37)$$

Eqs. (35), (36) and (37) are deduced from general Eq. (22) reminded below

$$\alpha_n = \frac{(2l+1)}{n} \times Z \left(1 - \frac{f_1({}^1L^e)}{Z} \right).$$

1. for the np^2 states

$$\alpha_2(0) = \frac{3}{2} Z \left(1 - \frac{93}{256} \times \frac{1}{Z} \right) = \frac{3}{2} Z \left(1 - f_1({}^1D^e) \times \frac{1}{Z} \right) \Rightarrow f_1({}^1D^e) = \frac{93}{256}. \quad (38)$$

2. for the nd^2 states

$$\alpha_3(0) = \frac{5}{3} Z \left(1 - \frac{2379}{6144} \times \frac{1}{Z} \right) = \frac{5}{3} Z \left(1 - f_1({}^1G^e) \times \frac{1}{Z} \right) \Rightarrow f_1({}^1G^e) = \frac{2379}{6144}. \quad (39)$$

3. for the nf^2 states

$$\alpha_4(0) = \frac{7}{4} Z \left(1 - \frac{26333}{65536} \times \frac{1}{Z} \right) = \frac{7}{4} Z \left(1 - f_1({}^1I^e) \times \frac{1}{Z} \right) \Rightarrow f_1({}^1I^e) = \frac{26333}{65536}. \quad (40)$$

Let us use approximately

$$f_1({}^1D^e) = \frac{93}{256} = 0.36328; \quad f_1({}^1G^e) = \frac{2379}{6144} = 0.38721; \quad f_1({}^1I^e) = \frac{26333}{65536} = 0.40181. \quad (41)$$

Using these values and Eqs. (13) and (14), the total energies of the doubly (n^2) excited states of the helium isoelectronic sequence are expressed explicitly as follows

1. For the np^2 doubly excited states, $l = 1$; $f_1({}^1D^e) = 0.36328$

$$E(np^2) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - \frac{0.36328}{Z} - \frac{0.36328 \times (Z-1)}{Z^2(2n-3)} - \frac{0.36328 \times Z}{Z^3} \right)^2 \right\}. \quad (42)$$

2. For the nd^2 doubly excited states, $l = 2$; $f_1({}^1G^e) = 0.38721$

$$E(nd^2) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - \frac{0.38721}{Z} - \frac{0.38721 \times (2Z-5/2)}{Z^2(n-1)} - \frac{0.38721 \times (2Z-3/2)}{Z^3} \right)^2 \right\}. \quad (43)$$

3. For the nf^2 doubly excited states, $l = 3$; $f_1({}^1I^e) = 0.40181$

$$E(nf) = -\frac{Z^2}{n^2} \times \left\{ 1 + \left(1 - \frac{0.40181}{Z} - \frac{0.40181 \times (3Z-3)}{Z^2(2n-5)} - \frac{0.40181 \times (3Z-2)}{Z^3} \right)^2 \right\}. \quad (44)$$

At this stage, one can appreciate positively the merit of the variational procedure of the SCUNC formalism as energies of the doubly (n^2) excited states of the helium isoelectronic sequence can be easily calculated directly without using any computational code. The total energies of the doubly (np^2), (nd^2) and (nf^2) excited states of the helium isoelectronic sequence with $2 \leq Z \leq 10$ and $2 \leq n \leq 20$ obtained in the present calculations are listed in Tables 1, 2 and 3 respectively using Eqs. (42) to (44), list. In Table 4, the present results for total

energies of the doubly excited np^2 ${}^1D^e$ ($n = 2 - 10$) states of He-like systems ($Z = 3 - 10$) are compared with those obtained from the semi-empirical procedure of the SCUNC formalism by Sakho *et al.*, [12], the complex rotation computations (CRC) by Ho and Bhatia [1], the variational method of Hylleraas by Biaye *et al.*, [4], the method of computing double sums over the total hydrogen spectrum (CDSHS) by Ivanov and Safronova [5] and those obtained by Roy *et al.*, [6] who applied the density functional theory (DFT). Comparison

shows that the present SCUNC results are generally in good agreement with those obtained by the aforementioned works. It should be mentioned that, for the $4p^2$ state with $Z = 10$, the largest energy difference between the present SCUNC result (11.9323 Ryd) and the accurate complex rotation calculation (11.9447 Ryd) of Ho and Bhatia [1] is equal to 0.0124 Ryd. In addition, it can be seen that both the present variational procedure and the semi-empirical procedure [12] of the SCUNC method provides accurate results comparing well with each other and with literature computational values [1-6]. Indeed, within the framework of the semi-empirical procedure, the screening constants are more easily evaluated from experimental data incorporating all electronic correlations effects (such as electron-electron interactions, nuclear volume effects (the larger the nucleus, the closer the electrons are to the core atmosphere and the more intense is their Coulomb repulsion, etc.), along with all relativistic effects (variation of the mass of electrons with velocity, spin-spin interaction, spin-orbit interaction, etc.). Table 5, shows a comparison of the present SCUNC results of total energies of the doubly excited $nd^2\ ^1G^e$ ($n = 3-8$) states of the He-like systems ($Z = 3-10$) with those obtained by Sakho *et al.*, [12], Bachau *et al.*, [7] who applied the Feshbach projection operators (FPO) formalism, of Biaye *et al* [4], Ivanov and Safronova [5] and with the data obtained by Roy *et al.*, [6]. The agreements between the calculations are seen to be good. It should be mentioned the very good agreement between the present calculations and those of Bachau *et al.*, [7] for the $3d^2$ level. For $Z = 10$, the SCUNC prediction at 20.5203 Ryd agree excellently with the Feshbach result of Bachau *et al.*, [7] equals to 20.5200 Ryd with an energy difference at 0.003 Ryd in absolute value. Table 6 lists the present SCUNC results for

total energies of the doubly excited $n\ell^2\ ^1I^e$ ($n = 2 - 10$) states of He-like systems compared with those obtained by Sakho *et al.*, [12], Biaye *et al.*, [4], and by Ho [8] who applied the method of complex rotation. A comparative reading of the results recorded in this table shows a good agreement between the present SCUNC results and those of the listed literature data for the $4\ell^2$ state. Overall, the good agreements between the present calculations and the various *ab initio* results for the doubly np^2 , nd^2 and $n\ell^2$ excited states of the He-like ions ($Z = 2-10$), justify the validity of the present variational procedure of the Screening Constant by Unit Nuclear Charge formalism. It should be mentioned that, calculations are directly obtained from analytical formulae in contrast with all the *ab initio* methods cited in this paper. In Tables 7 and 8, the present SCUNC results for the excitation energies of the doubly excited $np^2\ ^1D^e$ ($n = 2 - 5$) and $nd^2\ ^1G^e$ ($n = 3 - 5$) states of some He-like systems ($Z = 2 - 5$) are listed. Comparisons are done with the CRM results of Ho and Bhatia [1], the data from the discretization technique (DT) of Macias *et al.* [1], the values from the time-dependent variation perturbation theory (TVPT) of Ray and Mukherjee [11], the DFT data of Roy *et al.*, [6], the FOP values of Bhatia [20] and of Bachau *et al.*, [7] and with the CRC results of Lindroth [3] and of Ho and Callaway [3]. Comparisons indicate that the present SCUNC calculations agree well with the cited literature computations. This demonstrates again the validity of the variational procedure of the SCUNC formalism. Tables 9, lists present SCUNC values for the excitation energies of the doubly excited $n\ell^2\ ^1I^e$ states ($n = 4 - 7$) of the He-like systems ($Z = 2-5$). Here, no literature data have been found for comparison. The quoted SCUNC data are then good guideline for the doubly $n\ell^2\ ^1I^e$ excited states of the He-like systems investigated.

Table 1. Total energies of doubly $(np^2\ ^1D^e)$ excited states of He-like systems ($Z = 2-10$). Energies are expressed in Rydberg units. 1 Ryd = 13.60569 eV.

Z	2	3	4	5	6	7	8	9	10
np^2	-E	-E	-E	-E	-E	-E	-E	-E	-E
$2p^2$	1.4054	3.5421	6.6788	1.8155	15.9523	22.0890	29.2257	373624	46.4991
$3p^2$	0.6605	1.6587	3.1041	4.9951	7.3309	10.1115	13.3367	17.0064	21.1207
$4p^2$	0.3758	0.9429	1.7619	2.8315	4.1514	5.7214	7.5417	9.6119	11.9323
$5p^2$	0.2417	0.6062	1.1319	1.8181	2.6645	3.6710	4.8376	6.1642	7.6509
$6p^2$	0.1683	0.4220	0.7878	1.2649	1.8533	2.5529	3.3637	4.2856	5.3186
$7p^2$	0.1239	0.3106	0.5795	0.9304	1.3630	1.8773	2.4733	3.1509	3.9101
$8p^2$	0.0949	0.2380	0.4441	0.7129	1.0443	1.4382	1.8946	2.4136	2.9951
$9p^2$	0.0751	0.1882	0.3512	0.5636	0.8255	1.1369	1.4976	1.9077	2.3673
$10p^2$	0.0609	0.1526	0.2846	0.4567	0.6689	0.9212	1.2134	1.5457	1.9180
$11p^2$	0.0503	0.1261	0.2353	0.3761	0.5530	0.7615	1.0031	1.2777	1.5854
$12p^2$	0.0423	0.1060	0.1977	0.3174	0.4648	0.6400	0.8430	1.0738	1.3324
$13p^2$	0.0361	0.0904	0.1686	0.2705	0.3961	0.5454	0.7444	0.9151	1.1354
$14p^2$	0.0310	0.0779	0.1454	0.2333	0.3416	0.4704	0.6196	0.7892	0.9791
$15p^2$	0.0271	0.0679	0.1266	0.2032	0.2976	0.4098	0.5398	0.6875	0.8530
$16p^2$	0.0238	0.0597	0.1113	0.1787	0.2616	0.3602	0.4744	0.6043	0.7498
$17p^2$	0.0211	0.0529	0.0986	0.1583	0.2318	0.3191	0.4203	0.5353	0.6642
$18p^2$	0.0188	0.0472	0.0880	0.1412	0.2068	0.2847	0.3749	0.4775	0.5925
$19p^2$	0.0169	0.0424	0.0790	0.1267	0.1856	0.2555	0.3365	0.4286	0.5318
$20p^2$	0.0152	0.0382	0.0713	0.1144	0.1675	0.2306	0.3037	0.3869	0.4800

Table 2. Total energies of doubly ($nd^2\ ^1G^e$) excited states of He-like systems ($Z = 2-10$). Energies are expressed in Rydberg units. 1 Ryd = 13.60569 eV.

Z	2	3	4	5	6	7	8	9	10
nd ²	-E	-E	-E	-E	-E	-E	-E	-E	-E
3d ²	0.6113	1.5345	2.9079	4.7291	7.0000	9.7100	12.8684	1.4720	20.5203
4d ²	0.3514	0.8842	1.6716	2.7114	4.0026	5.5447	7.3372	9.3802	11.6734
5d ²	0.2274	0.5727	1.0815	1.7520	2.5834	3.5754	4.7278	6.0404	7.5132
6d ²	0.1590	0.4006	0.7560	1.2237	1.8032	2.4942	3.2966	4.2102	5.2352
7d ²	0.1173	0.2958	0.5578	0.9025	1.3292	1.8380	2.4286	3.1009	3.8549
8d ²	0.0901	0.2273	0.4284	0.6929	1.0202	1.4103	1.8630	2.3783	2.9562
9d ²	0.0714	0.1800	0.3393	0.5486	0.8075	1.1161	1.4741	1.8816	2.3386
10d ²	0.0579	0.1461	0.2753	0.4451	0.6550	0.9052	1.1954	1.5257	1.8960
11d ²	0.0479	0.1209	0.2279	0.3683	0.5419	0.7488	0.9888	1.2619	1.5681
12d ²	0.0403	0.1018	0.1917	0.3098	0.4558	0.6297	0.8315	1.0611	1.3185
13d ²	0.0344	0.0868	0.1635	0.2642	0.3887	0.5369	0.7089	0.9046	1.1240
14d ²	0.0297	0.0749	0.1411	0.2280	0.3354	0.4632	0.6116	0.7804	0.9696
15d ²	0.0259	0.0653	0.1230	0.1987	0.2923	0.4037	0.5330	0.6801	0.8449
16d ²	0.0228	0.0574	0.1082	0.1747	0.2570	0.3550	0.4686	0.5979	0.7429
17d ²	0.0202	0.0509	0.0959	0.1549	0.2278	0.3146	0.4153	0.5298	0.6582
18d ²	0.0180	0.0454	0.0856	0.1382	0.2032	0.2807	0.3705	0.4727	0.5873
19d ²	0.0162	0.0408	0.0768	0.1241	0.1825	0.2520	0.3326	0.4244	0.5272
20d ²	0.0146	0.0368	0.0694	0.1120	0.1647	0.2275	0.3003	0.3831	0.4759

Table 3. Total energies doubly excited of ($nf^2\ ^1F^e$) states of He-like systems ($Z = 2-10$). Energies are expressed in Rydberg units. 1 Ryd = 13.60569 eV.

Z	2	3	4	5	6	7	8	9	10
nf ²	-E	-E	-E	-E	-E	-E	-E	-E	-E
4f ²	0.3193	0.8170	1.5798	2.5967	3.8659	5.3866	7.1582	9.1804	11.4530
5f ²	0.2063	0.5406	1.0410	1.7044	2.5294	3.5154	4.6620	5.9690	7.4364
6f ²	0.1453	0.3809	0.7321	1.1965	1.7733	2.4618	3.2619	4.1733	5.1962
7f ²	0.1077	0.2821	0.5416	0.8844	1.3097	1.8171	2.4065	3.0777	3.8307
8f ²	0.0829	0.2171	0.4165	0.6767	1.0060	1.3954	1.8474	2.3620	2.9393
9f ²	0.0657	0.1722	0.3301	0.5385	0.7968	1.1048	1.4623	1.8694	2.3259
10f ²	0.0534	0.1398	0.2680	0.4370	0.6465	0.8962	1.1861	1.5161	1.8861
11f ²	0.0442	0.1158	0.2219	0.3617	0.5350	0.7415	0.9812	1.2541	1.5601
12f ²	0.0372	0.0974	0.1867	0.3043	0.4500	0.6237	0.8252	1.0546	1.3118
13f ²	0.0317	0.0831	0.1593	0.2595	0.3838	0.5318	0.7036	0.8991	1.1183
14f ²	0.0274	0.0718	0.1374	0.2240	0.3311	0.4588	0.6070	0.7756	0.9647
15f ²	0.0239	0.0626	0.1198	0.1952	0.2886	0.3999	0.5290	0.6759	0.8407
16f ²	0.0210	0.0550	0.1054	0.1717	0.2538	0.3516	0.4651	0.5943	0.7391
17f ²	0.0186	0.0488	0.0934	0.1522	0.2249	0.3116	0.4121	0.5266	0.6519
18f ²	0.0166	0.0435	0.0833	0.1358	0.2007	0.2780	0.3677	0.4098	0.5843
19f ²	0.0149	0.0391	0.0748	0.1219	0.1802	0.2496	0.3301	0.4218	0.5245
20f ²	0.0135	0.0353	0.0676	0.1101	0.1626	0.2253	0.2980	0.3807	0.4735

Table 4. Comparison of the present calculations on total energies of the doubly $np^2\ ^1D^e$ ($n = 2-10$) excited states of He-like systems ($Z = 2 - 10$) with available literature values. All results are expressed in Rydberg (Ryd) units: 1Ryd = 13.60569 eV.

		Z								
		2	3	4	5	6	7	8	9	10
2p ²	-E ^p	1.4054	3.5421	6.6788	10.8155	15.9523	22.0890	29.2257	37.3624	46.4991
	-E ^a	1.4053	3.5419	6.6785	10.8152	15.9518	22.0884	29.2250	37.3617	46.4983
	-E ^b	1.4039	3.5412	6.6749	10.8070	15.9383	22.0691	29.1997	37.3300	46.4603
	-E ^c	1.4100	3.5567	6.6989	10.8391	15.9781	22.1163	29.2541	37.3915	46.5286
	-E ^d	1.4270	3.5567	6.6864	10.8161	15.9457	22.0754	29.2051	37.3348	46.4645
3p ²	-E ^e		3.5118	6.6550	10.7976					
	-E ^p	0.6605	1.6587	3.1041	4.9951	7.3309	10.1115	13.3367	17.0064	21.1207
	-E ^a	0.6755	1.6627	3.0943	4.9703	7.2908	10.0557	13.2651	16.9189	21.0172
	-E ^b	0.6863	1.6843	3.1270	5.0141	7.3458	10.1220	13.3427	17.0078	21.1173
	-E ^c	0.6372	1.6027	3.0158	4.8786	7.1911	9.9548	13.1696	16.8356	20.9529
4p ²	-E ^d	0.6607	1.6252	3.0342	4.8875	7.1854	9.9276	13.1144	16.7455	20.8211
	-E ^e		1.6042	3.0204	4.8808					
	-E ^p	0.3758	0.9429	1.7619	2.8315	4.1514	5.7214	7.5417	9.6119	11.9323
	-E ^a	0.3957	0.9615	1.7773	2.8431	4.1590	5.7248	7.5406	9.6065	11.9223
	-E ^b		0.9648	1.7832	2.8517	4.1703	5.7388	7.5576	9.6262	11.9447
5p ²	-E ^c	0.3597	0.8993	1.6860	2.7211	4.0052	5.5389	7.3226	9.3564	11.6403
	-E ^d		0.9099	1.7097	2.7594					
	-E ^p	0.2417	0.6062	1.1319	1.8181	2.6645	3.6710	4.8376	6.1642	7.6509
	-E ^a	0.2595	0.6257	1.1519	1.8381	2.6843	3.6904	4.8566	6.1828	7.6690

		Z								
		2	3	4	5	6	7	8	9	10
	$-E^c$		0.5844	1.0973	1.7701					
6p ²	$-E^p$	0.1683	0.4220	0.7878	1.2649	1.8533	2.5529	3.3637	4.2856	5.3186
7p ²	$-E^p$	0.1239	0.3106	0.5795	0.9304	1.3630	1.8773	2.4733	3.1509	3.9101
8p ²	$-E^p$	0.0949	0.2380	0.4441	0.7129	1.0443	1.4382	1.8946	2.4136	2.9951
9p ²	$-E^p$	0.0751	0.1882	0.3512	0.5636	0.8255	1.1369	1.4976	1.9077	2.3673
10p ²	$-E^p$	0.0609	0.1526	0.2846	0.4567	0.6689	0.9212	1.2134	1.5457	1.9180

^pPresent work, variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^aSakho *et al.*, (2010), Semi-empirical procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^bHo and Bhatia [1], complex rotation method.

^cBiaye *et al* [4], variational method of Hylleraas.

^dIvanov and Safronova [5], method of computing double sums over the total hydrogen spectrum.

^eRoy *et al.*, [6], density functional theory.

Table 5. Comparison of the present calculations on total energies of the doubly $nd^2\ ^1G^e$ ($n = 3-10$) excited states of He – like systems ($Z = 2-10$) with available literature values. All results are expressed in Rydberg (Ryd) units: $1\text{Ryd} = 13.60569\text{ eV}$.

		Z								
		2	3	4	5	6	7	8	9	10
	$-E^p$	0.6113	1.5345	2.9079	4.7291	7.0000	9.7100	12.8684	16.4720	20.5203
	$-E^a$	0.6104	1.5487	2.9314	4.7585	7.0301	9.7462	12.9067	16.5116	20.5610
3d ²	$-E^b$	0.6166	1.5538	2.9320	4.7540	7.0180	9.7280	12.8820	16.4800	20.5200
	$-E^c$	0.6309	1.5837	2.9763	4.8106	7.0876	9.8079	12.9719	16.5797	20.6316
	$-E^d$	0.6304	1.5618	2.9378	4.7581	7.0229	9.7320	12.8859	16.4840	20.5266
	$-E^e$	0.5850	1.5247	2.9086	4.7366					
	$-E^p$	0.3514	0.8842	1.6716	2.7114	4.0026	5.5447	7.3372	9.3802	11.6734
4d ²	$-E^a$	0.3567	0.8950	1.6834	2.7217	4.0100	5.5484	7.3367	9.3750	11.6634
	$-E^c$	0.3597	0.8993	1.6859	2.7210	4.0051	5.5387	7.3223	9.3559	11.6699
	$-E^e$	0.3458	0.8865	1.6772	2.7177					
	$-E^p$	0.2274	0.5727	1.0815	1.7520	2.5834	3.5754	4.7278	6.0404	7.5132
5d ²	$-E^a$	0.2337	0.5823	1.0909	1.7594	2.5880	3.5766	4.7252	6.0338	7.5024
	$-E^c$	0.2254	0.5743	1.0832	1.7521					
	$-E^p$	0.1590	0.4006	0.7560	1.2237	1.8032	2.4942	3.2966	4.2102	5.2352
6d ²	$-E^c$		0.4013	0.7557	1.2211					
	$-E^p$	0.1173	0.2958	0.5578	0.9025	1.3292	1.8380	2.4286	3.1009	3.8549
	$-E^e$		0.2848	0.5566	0.8990					
8d ²	$-E^p$	0.0901	0.2273	0.4284	0.6929	1.0202	1.4103	1.8630	2.3783	2.9562
9d ²	$-E^p$	0.0714	0.1800	0.3393	0.5486	0.8075	1.1161	1.4741	1.8816	2.3386
10d ²	$-E^p$	0.0579	0.1461	0.2753	0.4451	0.6550	0.9052	1.1954	1.5257	1.8960

^pPresent work, variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^aSakho *et al.*, [12], semi-empirical procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^bBachau *et al.*, [7], Feshbach operators projection formalism.

^cBiaye *et al.*, [4], variational method of Hylleraas.

^dIvanov and Safronova [5], method of computing double sums over the total hydrogen spectrum.

^eRoy *et al.*, [6], density functional theory.

Table 6. Comparison of the present calculations on total energies of the doubly $nf^2\ ^1F^e$ ($n = 4 - 10$) excited states of He – like systems ($Z = 2 - 10$) with available literature values. All results are expressed in Rydberg (Ryd) units: $1\text{Ryd} = 13.60569\text{ eV}$.

		Z								
		2	3	4	5	6	7	8	9	10
	$-E^p$	0.3193	0.8170	1.5798	2.5967	3.8659	5.3866	7.1582	9.1804	11.4530
4f ²	$-E^a$	0.3238	0.8346	1.5955	2.6063	3.8671	5.3780	7.1388	9.1496	11.4105
	$-E^b$	0.3591	0.8978	1.6828	2.7155	3.9964	5.5262	7.3049	9.3330	11.6100
	$-E^c$	0.3408								
5f ²	$-E^p$	0.2063	0.5406	1.0410	1.7044	2.5294	3.5154	4.6620	5.9690	7.4364
6f ²	$-E^p$	0.1453	0.3809	0.7321	1.1965	1.7733	2.4618	3.2619	4.1733	5.1962
7f ²	$-E^p$	0.1077	0.2821	0.5416	0.8844	1.3097	1.8171	2.4065	3.0777	3.8307
8f ²	$-E^p$	0.0829	0.2171	0.4165	0.6767	1.0060	1.3954	1.8474	2.3620	2.9393
9f ²	$-E^p$	0.0657	0.1722	0.3301	0.5385	0.7968	1.1048	1.4623	1.8694	2.3259
10f ²	$-E^p$	0.0534	0.1398	0.2680	0.4370	0.6465	0.8962	1.1861	1.5161	1.8861

^pPresent work, variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^aSakho *et al.*, [12], semi-empirical procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^bBiaye *et al.*, [4], variational method of Hylleraas.

^cHo [8], complex rotation method.

Table 7. Comparison of the present calculations on the variational calculation of the excitation energies of the doubly excited $np^2\ ^1D^e$ states ($n = 2 - 5$) of the He-like systems with some theoretical results available in the literature consulted for $2 \leq Z \leq 5$. The ground state energies from Frankowski and Pekeris [21] are used in this work and they are the following in atomic units: -7.27991 (Li^+), -13.65556 (Be^{2+}) and -22.03097 (B^{3+}). All the results are expressed in a. u with $1 a. u = 2Ryd$; $1Ryd = 13.60569 eV$.

Z	nl	Total energy ($-E$, a. u)	Excitation energy (ΔE , a. u)	
			Present work	Literature values
2	2p2p	0.702 71	-	
	3p3p	0.330 26	-	
	4p4p	0.187 90	-	
	5p5p	0.120 85	-	
	2p2p	1.771 07 1.770 61 ^b	5.5088	5.5093 ^b , 5.5192 ^c , 5.5080 ^g , 5.5146 ^c , 5.5243 ^f
3	3p3p	0.829 37 0.796 39 ^b	6.4505	6.4835 ^b , 6.4842 ^b , 6.4671 ^d
	4p4p	0.471 47	6.8085	6.8128 ^d , 6.8250 ^f
	5p5p	0.303 11	6.9768	6.9708 ^d , 6.9877 ^f
	2p2p	3.339 43 3.337 43 ^b	10.3161	10.3181 ^b , 10.3319 ^c , 10.3281 ^f , 10.3248 ^e , 10.3576 ^d
	3p3p	1.552 09 1.498 89	12.1034	12.1567 ^b , 12.1454 ^f , 12.1576 ^b , 12.1323 ^d
4	4p4p	0.880 93	12.7746	12.7882 ^d , 12.8007 ^f
	5p5p	0.565 98	13.0896	13.1658 ^d , 13.1068 ^f
	2p2p	5.407 79 5.403 48 ^b	16.6232	16.6275 ^b , 16.6438 ^e , 16.6352 ^c , 16.6783 ^d , 16.6322 ^f
	3p3p	2.497 54 2.423 37	19.5334	19.6079 ^b , 19.6080 ^h , 19.5906 ^f , 19.5992 ^d
	4p4p	1.415 73	20.6152	20.6382 ^d , 20.6512 ^f
5p5p	0.909 07	21.1219	21.1311 ^d , 21.1459 ^f	

^aPresent work, variational procedure of the Screening Constant by Unit Nuclear. Charge (SCUNC) method.

^bHo and Bhatia [1], complex rotation method.

^cMacias et al., [9], discretization technique.

^dRay and Mukherjee [11], time-dependent variation perturbation theory.

^eConneely and Lipsky [10], truncated diagonalization method.

^fRoy et al., [6], density functional theory.

^gBhatia [20], Feshbach projection operators formalism.

^hBachau et al., [7], Feshbach projection operators formalism.

Table 8. Comparison of the present calculations on the excitation energies of the doubly excited $nd^2\ ^1G^e$ states ($n = 3-7$) of the He-like systems with some theoretical results available in the literature consulted for $2 \leq Z \leq 5$. The ground state energies from Frankowski and Pekeris [21] are used in this work and they are the following in atomic units (a. u): -7.27991 (Li^+), -13.65556 (Be^{2+}) and -22.03097 (B^{3+}). All the results are expressed in a. u with $1 a. u = 2Ryd$; $1Ryd = 13.60569 eV$.

Z	nl	Total energy ($-E$, a. u)	Excitation energy (ΔE , a. u)	
			Present work	Literature values
2	3d3d	0.305 67 0.307 12 ^b	2.5981	2.5963 ^b , 2.5967 ^c , 2.5954 ^d 2.7085 ^f
	4d4d	0.17572	2.7280	
	5d5d	0.11370	2.7900	
	6d6d	0.07949	2.8242	2.7807 ^f
	7d7d	0.05866	2.8451	
	3d3d	0.76726 0.776 90 ^d	6.5126	6.5030 ^d , 6.5176 ^c , 6.5025 ^f
3	4d4d	0.442 08	6.8378	6.8367 ^c , 6.8199 ^f
	5d5d	0.28637	6.9935	6.9928 ^c , 6.9757 ^f
	6d6d	0.20033	7.0796	7.0793 ^c
	7d7d	0.14790	7.1320	7.1320 ^c
	3d3d	1.453 97 1.466 00 ^d	12.2016	12.1896 ^d , 12.1915 ^f 12.2013 ^c
	4d4d	0.835 79	12.8178	12.8170 ^c , 12.7982 ^f
4	5d5d	0.540 76	13.1148	13.1139 ^c , 13.1703 ^f
	6d6d	0.378 00	13.2776	13.2777 ^c
	7d7d	0.27893	13.3766	13.3773 ^c
	3d3d	2.364 57 2.377 00 ^d	19.6664	19.6540 ^d , 19.6627 ^c 19.6583 ^f
	4d4d	1.35572	20.6752	20.6721 ^c , 20.6509 ^f
	5d5d	0.87601	21.1550	21.1549 ^c , 21.1331 ^f

Z	nl	Total energy ($-E$, a. u.)	Excitation energy (ΔE , a. u.)	
			Present work	Literature values
	6d6d	0.61185	21.4191	21.4204 ^c
	7d7d	0.45125	21.5797	21.5814 ^e

^aPresent work, variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

^bLindroth [2], complex rotation method.

^cHo and Callaway [3], complex rotation method.

^dBachau *et al.*, [7], Feshbach projection operators formalism.

^eRoy *et al.*, [6], density functional theory.

^fRay and Mukherjee [11], time-dependent variation perturbation theory.

Table 9. Comparison of the present calculations on the excitation energies of the doubly excited $nl^2\ ^1F^\pi$ states ($n = 4 - 7$) of the helium-like systems with some theoretical results available in the literature consulted for $2 \leq Z \leq 5$. The ground state energies from Frankowski and Pekeris [21] are used in this work and they are the following in (a. u.): -7.27991 (Li^+), -13.65556 (Be^{2+}) and -22.03097 (B^{3+}). All the results are expressed in a. u with $1a. u = 2Ryd$; $1Ryd = 13.60569 eV$.

Z	nl	Total energy ($-E$, a. u.)	Excitation energy (ΔE , a. u.)	
			Present work	Literature values
2	4f4f	0.155 97		
	5f5f	0.103 15		
	6f6f	0.072 68		
	7f7f	0.053 83		
	4f4f	0.408 48	6.8714	-
3	5f5f	0.270 31	7.0096	-
	6f6f	0.190 45	7.0895	-
	7f7f	0.141 06	7.1388	-
	4f4f	0.796 29	12.8593	-
4	5f5f	0.523 05	13.1325	-
	6f6f	0.367 33	13.2882	-
	7f7f	0.271 56	13.3840	-
	4f4f	1.305 18	20.7258	-
5	5f5f	0.854 89	21.1761	-
	6f6f	0.599 62	21.4313	-
	7f7f	0.442 99	21.5880	-

^aPresent work, variational procedure of the Screening Constant by Unit Nuclear Charge (SCUNC) method.

4. Conclusion

In this work, the variational procedure of the Screening constant by unit nuclear charge (SCUNC) method has been applied for the first time to the calculations of total energies and excitation energies of the doubly $mp^2\ D^e$, $nd^2\ G^e$ and $nl^2\ I^e$ excited states of the He-like systems ($Z = 2 - 10$). A new correlated wave function adapted to the correct description of the electron-electron correlations phenomena in the doubly excited nl^2 states of the He-like systems has been constructed. The good results obtained in this work indicate the possibility to apply the variational procedure of the SCUNC method to the treatment of atomic spectra in two electron systems and probably in more complex atomic systems. Study is in such direction.

Appendix

Detail in the calculation of the screening constant for the $np^2\ ^1D^e$ levels (that for the $nd^2\ ^1G^e$ and $nl^2\ ^1I^e$ levels are of similar)

$$E(\alpha) \iint d^3r_1 d^3r_2 \langle \Psi(\alpha) | \vec{r}_1, \vec{r}_2 \rangle \times \langle \vec{r}_1, \vec{r}_2 | \Psi(\alpha) \rangle = \iint d^3r_1 d^3r_2 \langle \Psi(\alpha) | \vec{r}_1, \vec{r}_2 \rangle \hat{H} \langle \vec{r}_1, \vec{r}_2 | \Psi(\alpha) \rangle$$

That means

The eigenvalue $E(\alpha_n)$ of the doubly nl^2 excited state is given by

$$E(\alpha_n) = \langle \hat{H} \rangle(\alpha_n) = \frac{\langle \Psi(\alpha_n) | \hat{H} | \Psi(\alpha_n) \rangle}{\langle \Psi(\alpha_n) | \Psi(\alpha_n) \rangle} \quad (A.1)$$

In this equation, the correlated wave function and the Hamiltonian are expressed as follows

$$\Psi(r_1, r_2, \alpha_n) = (r_1, r_2)^l \exp -\alpha_n (r_1 + r_2) . \quad (A.2)$$

$$\hat{H} = -\frac{1}{2} \Delta_1 - \frac{1}{2} \Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} . \quad (A.3)$$

Using the relation satisfy by the basis $|\vec{r}_1, \vec{r}_2\rangle$:

$$\iint d^3r_1 d^3r_2 |\vec{r}_1, \vec{r}_2\rangle \langle \vec{r}_1, \vec{r}_2| = 1,$$

equation (A.1) provides

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

and

$$N E(\alpha) = \iint d^3r_1 d^3r_2 \Psi(r_1, r_2, \alpha) \hat{H} \Psi^*(r_1, r_2, \alpha) \quad (\text{A.4})$$

with

$$N = \iint d^3r_1 d^3r_2 |\Psi(r_1, r_2, \alpha)|^2 \quad (\text{A.5})$$

The constant of normalization.

To facilitate the resolution of (A.4), let us make the change of the following usual variables then in elliptic coordinates

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

$$d\tau = d^3r_1 d^3r_2 = 2\pi^2 (s^2 - t^2) u ds dt du.$$

Eq. (A.4) is then rewritten in elliptic coordinate as follows

$$N E(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 + \left(\frac{\partial \Psi}{\partial t} \right)^2 + \left(\frac{\partial \Psi}{\partial u} \right)^2 \right] + 2 \left(\frac{\partial \Psi}{\partial u} \right) \times \left[s(u^2 - t^2) \frac{\partial \Psi}{\partial s} + \right. \right. \\ \left. \left. + t(s^2 - u^2) \frac{\partial \Psi}{\partial t} \right] - \Psi^2 [4Zsu - s^2 + t^2] \right\} \quad (\text{A.6})$$

The correlated wave function is in the

$$\Psi(s, t, \alpha_n) = \frac{1}{4} (s^2 - t^2) \exp(-\alpha_n s) \quad (\text{A.7})$$

The wave function does not depend on u , Eq. (A.6) is reduced to

$$N E(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt \left\{ u(s^2 - t^2) \times \left[\left(\frac{\partial \Psi}{\partial s} \right)^2 - \left(\frac{\partial \Psi}{\partial t} \right)^2 \right] - \Psi^2 [4Zsu - s^2 + t^2] \right\} \quad (\text{A.8})$$

The above expression can be shared into three parts

$$N E(\alpha) = E_1(\alpha) + E_2(\alpha) + E_3(\alpha) \quad (\text{A.9})$$

with

$$E_1(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt u(s^2 - t^2) \times \left(\frac{\partial \Psi}{\partial s} \right)^2 \quad (\text{A.10})$$

$$E_2(\alpha) = \int_0^\infty ds \int_0^s du \int_0^u dt u(s^2 - t^2) \times \left(\frac{\partial \Psi}{\partial t} \right)^2 \quad (\text{A.11})$$

$$E_3(\alpha) = - \int_0^\infty ds \int_0^s du \int_0^u dt [4Zsu - s^2 + t^2] \Psi^2 \quad (\text{A.12})$$

$$N = \int_0^\infty ds \int_0^s du \int_0^u dt u(s^2 - t^2) \times \Psi^2 \quad (\text{A.13})$$

Let us put $\alpha_n = \alpha$ for sake of simplification. Using Eq. (A.7), Eq. (A.10) gives

$$\begin{aligned}
E_1(\alpha) &= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \int_0^u dt \left[(4s^4 - 4\alpha s^5 + \alpha^2 s^6)u + (-4s^2 + 8\alpha s^3 - 3\alpha^2 s^4)ut^2 \right. \\
&\quad \left. + (-4\alpha s + 3\alpha^2 s^2)ut^4 - \alpha^2 ut^6 \right] \\
E_1(\alpha) &= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \int_0^u dt \left[(4s^4 - 4\alpha s^5 + \alpha^2 s^6)u + (-4s^2 + 8\alpha s^3 - 3\alpha^2 s^4)ut^2 \right. \\
&\quad \left. + (-4\alpha s + 3\alpha^2 s^2)ut^4 - \alpha^2 ut^6 \right] \\
&= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \left[(4s^4 - 4\alpha s^5 + \alpha^2 s^6)u^2 + \left(-\frac{4}{3}s^2 + \frac{8}{3}\alpha s^3 - \alpha^2 s^4 \right)u^4 \right. \\
&\quad \left. + \left(-\frac{4}{5}\alpha s + \frac{3}{5}\alpha^2 s^2 \right)u^6 - \frac{1}{7}\alpha^2 u^8 \right] \\
&= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \left[\left(\frac{4}{3}s^7 - \frac{4}{3}\alpha s^8 + \frac{1}{3}\alpha^2 s^9 \right) + \left(-\frac{4}{15}s^7 + \frac{8}{15}\alpha s^8 - \frac{1}{5}\alpha^2 s^9 \right) \right. \\
&\quad \left. + \left(-\frac{4}{35}\alpha s + \frac{3}{35}\alpha^2 s^2 \right) - \frac{1}{63}\alpha^2 s^9 \right] \\
&= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \left[\left(\frac{1}{3} - \frac{1}{5} + \frac{3}{35} - \frac{1}{63} \right) \alpha^2 s^9 + \left(-\frac{4}{3} + \frac{8}{15} - \frac{4}{15} \right) \alpha s^8 + \left(\frac{4}{3} - \frac{4}{35} \right) s^7 \right] \\
&= \frac{1}{16} \int_0^\infty e^{-2\alpha s} ds \left[\frac{1344}{6615} \alpha^2 s^9 - \frac{288}{315} \alpha s^8 + \frac{16}{15} s^7 \right]
\end{aligned}$$

So, finally

$$E_1(\alpha) = \frac{84}{6615} \alpha^2 \int_0^\infty s^9 e^{-2\alpha s} ds - \frac{18}{315} \alpha \int_0^\infty s^8 e^{-2\alpha s} ds + \frac{1}{15} \int_0^\infty s^7 e^{-2\alpha s} ds$$

In the same way, Eq. (A.11) gives successively

$$\begin{aligned}
E_2(\alpha) &= \frac{1}{4} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \int_0^u dt \left[us^2 t^2 - ut^4 \right] \\
&= \frac{1}{4} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \int_0^u dt \left[us^2 t^2 - ut^4 \right] = \frac{1}{4} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \left[us^2 \int_0^u t^2 dt - u \int_0^u t^4 dt \right] \\
&= \frac{1}{4} \int_0^\infty e^{-2\alpha s} ds \int_0^s du \left[\frac{1}{3} u^4 s^2 - \frac{1}{5} u^6 \right] \\
&= \frac{1}{4} \int_0^\infty e^{-2\alpha s} ds \left[\frac{1}{15} s^7 - \frac{1}{35} s^7 \right]
\end{aligned}$$

$$= \frac{1}{4} \int_0^{\infty} e^{-2\alpha s} \left[\frac{4}{105} s^7 \right] ds = \frac{1}{105} \int_0^{\infty} s^7 e^{-2\alpha s} ds$$

Then

$$E_2(\alpha) = \frac{1}{105} \int_0^{\infty} s^7 e^{-2\alpha s} ds \quad (\text{A.14})$$

In addition, Eq. (A.12) gives

$$\begin{aligned} E_3(\alpha) &= -\frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \int_0^s du \int_0^u dt \left[(4Zs^5u - s^6) + (-8Zs^3u + 3s^4)t^2 + (4Zsu - 3s^2)t^4 + t^6 \right] \\ &= -\frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \int_0^s du \left[(4Zs^5u - s^6) \int_0^u dt + (-8Zs^3u + 3s^4) \int_0^u t^2 dt + (4Zsu - 3s^2) \int_0^u t^4 dt + \int_0^u t^6 dt \right] \\ &\quad + \frac{1}{5} (4Zsu - 3s^2) u^5 + \frac{1}{7} u^7 \Big] \\ &= -\frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \left[\left(4Zs^5 \int_0^s u^2 du - s^6 \int_0^s u du \right) + \left(-\frac{8}{3} Zs^3 \int_0^s u^4 du + s^4 \int_0^s u^3 du \right) + \left(\frac{4}{5} Zs \int_0^s u^6 du - \frac{3}{5} s^2 \int_0^s u^5 du \right) + \frac{1}{7} \int_0^s u^7 du \right] \\ &= -\frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \left[\left(\frac{4}{3} Zs^8 - \frac{1}{2} s^8 \right) + \left(-\frac{8}{15} Zs^8 + \frac{1}{4} s^8 \right) + \left(\frac{4}{35} Zs^8 - \frac{1}{10} s^8 \right) + \frac{1}{56} s^8 \right] \\ &= -\left[\frac{18}{315} Z - \frac{93}{4480} \right] \int_0^{\infty} s^8 e^{-2\alpha s} ds \\ E_3(\alpha) &= -\left[\frac{18}{315} Z - \frac{93}{4480} \right] \int_0^{\infty} s^8 e^{-2\alpha s} ds \quad (\text{A.15}) \end{aligned}$$

Finally, using (A.14), the normalization constant is equal to

$$\begin{aligned} N &= \frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \int_0^s du \int_0^u dt u \left[s^6 - 3s^4 t^2 + 3s^2 t^4 - t^6 \right] \\ &= \frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \int_0^s du \left[us^6 \int_0^u dt - 3us^4 \int_0^u t^2 dt + 3us^2 \int_0^u t^4 dt - u \int_0^u t^6 dt \right] \\ &= \frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \left[s^6 \int_0^s u^2 du - s^4 \int_0^s u^4 du + \frac{3}{5} s^2 \int_0^s u^6 du - \frac{1}{7} \int_0^s u^8 du \right] \\ &= \frac{1}{16} \int_0^{\infty} e^{-2\alpha s} ds \left[\frac{1}{3} s^9 - \frac{1}{5} s^9 + \frac{3}{35} s^9 - \frac{1}{63} s^9 \right] \end{aligned}$$

That means

$$N = \frac{84}{6615} \int_0^\infty s^9 e^{-2\alpha s} ds \quad (\text{A.16})$$

All the equations (A.13), (A.14), (A.15) and (A.16) are of the type

$$\int_0^\infty x^n e^{-ax} dx = \frac{1}{a} \frac{n!}{a^{n+1}} \quad (\text{A.17})$$

Using (A.17), Eqs. (A.13), (A.14), (A.15) and (A.16) are expressed as follows

$$\begin{cases} E_1(\alpha) = \frac{1}{2} \left(\frac{84}{6615} \alpha^2 \times \frac{9!}{(2\alpha)^{10}} - \frac{18}{315} \alpha \times \frac{8!}{(2\alpha)^9} + \frac{1}{15} \times \frac{7!}{(2\alpha)^8} \right) \\ E_2(\alpha) = \frac{1}{2} \left(\frac{1}{105} \times \frac{7!}{(2\alpha)^8} \right) \\ E_3(\alpha) = -\frac{1}{2} \left(\frac{18}{315} Z - \frac{93}{4480} \right) \times \frac{8!}{(2\alpha)^9} \\ N = \frac{1}{2} \left(\frac{84}{6615} \alpha^2 \times \frac{9!}{(2\alpha)^{10}} \right) \end{cases} \quad (\text{A.18})$$

To simplify, let us put introduce the constant K such as $KN = 1$. So:

$$K = 2 \left(\frac{6615}{84} \times \frac{(2\alpha)^{10}}{9!} \right)$$

Eqs. (A.18) are then simplified as follows

$$\begin{cases} KE_1(\alpha) = \frac{7}{24} \alpha^2 \\ KE_2(\alpha) = \frac{1}{24} \alpha^2 \\ KE_3(\alpha) = - \left(Z - \frac{93}{256} \right) \alpha \\ KN = 1 \end{cases} \quad (\text{A.19})$$

Using Eq. (A.19), the eigen energy (A.9) is expressed as follows

$$E(\alpha) = \frac{7}{24} \alpha^2 + \frac{1}{24} \alpha^2 - \left[Z - \frac{93}{256} \right] \alpha$$

As $\alpha = \alpha_n$, the preceding equation is expressed as follows

$$E(\alpha) = \frac{1}{3} \alpha_n^2 - \left[Z - \frac{93}{256} \right] \alpha_n \quad (\text{A.20})$$

Turning into account the Ritz variational principle

$$\left. \frac{E(\alpha)}{d\alpha} \right|_{\alpha=\alpha(0)} = 0 \quad (\text{A.21})$$

Eq. (A.20) gives for the $mp^2\ ^1D^e$ states

$$\alpha_2(0) = \frac{3}{2} \left(Z - \frac{93}{256} \right) = \frac{3}{2} Z \left(1 - \frac{93}{256} \times \frac{1}{Z} \right). \quad (\text{A.22})$$

This last equation corresponds to Eq. (27.a).

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