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Calculations of $2sns^{+1,3}S^e$, $2snp^{+1,3}P^0$, $2pnp^{+1,3}D^e$ Autoionizing States in Two-Electrons Systems Using a New Wave Function to Four Terms

Boubacar Sow, Youssou Gning, Malick Sow, Alassane Traore, Ahmadou Wagué

Department of Physics, Atoms Laser Laboratory, University Cheikh Anta Diop, Dakar, Senegal

Email address:
boubacar1.sow@ucad.edu.sn (B. Sow), gningyoussou@yahoo.fr (Y. Gning), malickitna@yahoo.fr (M. Sow), traalou07@yahoo.fr (A. Traore),
ahmadou.wague@ucad.edu.sn (A. Wagué)

Abstract: In this paper, we calculate energies for $2s3s^{+1,3}S^e$, $2s4s^{+1,3}S^e$, $2snp^{+1,3}P^0$ with n≤6 and $2p3p^{+1,3}D^e$, $2p4p^{+1,3}D^e$ autoionizing states of helium-like ions. These calculations are investigated using a new wave function correlated to four terms. Total energies calculations are performed between two electrons in He-isoelectronic series up to $Z = 10$, base on the Screening Constant by Unit Nuclear charge method in the framework of a variational procedure. The results obtained are in compliance with recent theoretical calculations.

Keywords: Autoionizing States, Wave Function Correlated, He-Isoelectronic, Screen Constant by Unit Nuclear Charge

1. Introduction

Currently in atomic physics the studies concerning the determination of the characteristics of the doubly excited states such as total energies, the total widths as well as the cross sections of autoionisation are of a great importance. These studies allowed the theorists and the experimenters to highlight the importance of the phenomena of electronic correlation in the doubly excited states of the atomic systems with two electrons. [1-6].

Many efforts were deployed in the last few years in the clarification of several theoretical methods for the description of the atomic systems with two electrons; it is still possible to make other studies in this field in order to test new theoretical methods which can contribute to a better understanding of the phenomena of electronic correlations. Within this framework that a new wave function of four special terms of Hylleraas forms type was developed to describe the atomic systems with two doubly excited He atom and He-like ions with $Z \leq$ 15 [7-8].

These kinds of wave functions of special shape are used for the calculation of energy to the ground state and use more terms [9-11]. They allowed also with the use of the variational method combined with the theory of the interaction of the configurations, to describe in a very satisfactory way some singulets states of the same valence (nl^2, nlnl' with n ≤ 4) doubly excited of helium and He atom and He-like ions with [12-15].

This work constitutes a generalization of the studies to several doubly excited singulets and triplets $2sns^{+1,3}S^e$, $2snp^{+1,3}P^0$ and $2pnp^{+1,3}D^e$ states of the same electrons valence by using a new wave function of special forms of hylleraas types to four terms.

2. Theory

The calculation of the energy of the fundamental state was an outstanding contribution for quantum mechanics. A method of calculating energies of the fundamental state of helium and the space part associated with the function of wave was proposed by Hylleraas in 1928. [16]

The Hylleraas method was applied successfully by himself in the calculation of the energy of the fundamental state of He atom and He-like ions. To expand this application to calculate the total energy of atomic systems in the doubly excited states

must seek new wave functions correlated $\psi(\vec{r}_1, \vec{r}_2)$ adapted to the description of those states.

The helium atom and its isoelectronic series are atomic systems with two electrons. By neglecting the relativistic effects (variation of the mass of the electrons with speed, interaction spin-spin, spin-orbit coupling) and magnetic effects (had with the electric currents generated by the orbital movements of the electrons), Hamiltonian associated with the two electrons (1) and (2) with He atom and He-like ions is written in the approximation of the infinitely heavy core (what supposes the motionless core):

$$H = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad \text{(in a.u)} \quad (1)$$

This equation can be put in the form:

$$H = H_1 + H_2 + W \quad (2)$$

In the equation (2), H and W respectively indicate the no disturbed Hamiltonian and it is given by the following relations:

$$H_1 + H_2 = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} \quad (3)$$

and

$$W = \frac{1}{r_{12}} \quad (4)$$

In these equations: Z is the nuclear charge

Δ_1 is the Laplacian with reference to the coordinates of the vector radius r_1 which detect the position of the electron 1.

Δ_2 Laplacian defines the coordinates of the vector radius r_2 which detect the position of the electron 2 and $r_{12} = |\vec{r}_1 - \vec{r}_2|$ inter- electronic distance. Moreover, the Schrödinger equation applied to He-like systems is then written:

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (5)$$

The existence of the term of disturbance (4) then makes impossible the exact resolution of the equation (5).

It is thus we used the variational method which is one of the techniques of calculation making it possible to provide approximate solutions to the resolution of the equation of Schrödinger applied to the atomic systems with two electrons. It is for this reason one is brought to implement an approximate method of calculating using a function of wave known as correlated Ψ of four terms which is given by:

$$\Psi(r_1, r_2, \alpha) = k\, P(r_1, r_2, \alpha) e^{-4(r_1 + r_2)} \quad (6)$$

with

$$P(r_1, r_2, \alpha) = c_1 + c_2(r_1 + r_2)(r_{12})^2 + c_3(r_1 - r_2) + z\alpha r_{12} \quad (7)$$

and

$$k = \left(\frac{\sqrt{2}}{2}\right)^{\left(n + \ell + \ell' \pm 2(-1)^S\right)} \quad (8)$$

C_1, C_2, C_3 are fixed parameters for the ground state and in the excited state and the Screening Constant α reflecting the effect exerted by the charges of the electrons on the nuclear charge. Z the nuclear charge.

The normalization constant.

$$N = \iint dr_1^3 dr_2^3 \left|\Psi(r_1, r_2, \alpha)\right|^2 \quad (9)$$

To facilitate the integration of the equation, one transforms the polar into elliptical coordinates and asked:

$s = (r_1 + r_2)$; $t = (r_1 - r_2)$; $u = r_{12}$ [17]. Based on these variable changes, the elementary volume element

$$d\tau = dr_1^3 dr_2^3 \quad (10)$$

is written:

$$d\tau = 2\pi^2 (s^2 - t^2)\, u\, ds\, dt\, du \quad (11)$$

The normalization constant and correlated wave function are reduced to the simple form:

$$N = \int_0^\infty ds \int_0^s du \int_0^u dt\, u\left(s^2 - t^2\right) \times \Psi^2 \quad (12)$$

$$\Psi(s,t,u) = \left(\frac{\sqrt{2}}{2}\right)^{\left(n + \ell + \ell' \pm 2(-1)^S\right)} \left[(c_1 + c_2 su^2 + c_3 t + zu\alpha)e^{-4S}\right] \quad (13)$$

General expressions of total energies $2s3s\ ^{+1,3}S^e$, $2s4s\ ^{+1,3}S^e$, $2snp\ ^{+1,3}P^0$, $2p3p\ ^{+1,3}D^e$ and $2p4p\ ^{+1,3}D^e$ singulets and triplets excited states of He-like ions.

To pass to the eigenvalues, equation (2) gives for the ground state

$$E(1S_0) = E_1^{(1)} + E_1^{(2)} + W_1 \quad (14)$$

Using the perturbation theory, one finds for the average value of the electron correlation term (2) to the first-order approximation [18].

$$W_1 = \frac{5}{4} Z\, E_H \quad (15)$$

With

$$E_H = \frac{1}{2}\alpha^2 m_0 c^2 \quad (16)$$

Let us rewrite the result (15) that provides the perturbation theory to the first-order approximation as follows:

$$W_1 = \left(\frac{5}{4Z}\right) Z^2 E_H \qquad (17)$$

Let us then put

$$\varepsilon_1 = \left(\frac{5}{4Z}\right) \qquad (18)$$

By use of equation (17), (18) can be written in the form

$$E(1S_0) = E_1^{(1)} + E_1^{(2)} + \varepsilon_1 Z^2 E_H + \varepsilon_2 Z^2 E_H + \varepsilon_3 Z^2 E_H + \varepsilon_4 Z^2 E_H + L + L\varepsilon_p Z^2 E_H \qquad (20)$$

That means

$$E(1S_0) = E_1^{(1)} + E_1^{(2)} + (\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + L + L\varepsilon_p + O(\varepsilon_v)) Z^2 E_H \qquad (21)$$

To a *q*-order approximation as elevated as possible, let us write (21) in the form

$$E(1S_0) = E_1^{(1)} + E_1^{(2)} + (\sum_{p=1}^{q} \varepsilon_p) Z^2 E_H \qquad (22)$$

Otherwise, taking into account the fact that,

$$E_1^{(1)} = E_1^{(2)} = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 \qquad (23)$$

equation (22) becomes

$$E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 + (\sum_{p=1}^{q} \varepsilon_p) Z^2 E_H \qquad (24)$$

Using (16), one gets from (23)

$$E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 + (\sum_{p=1}^{q} \varepsilon_p) \frac{1}{2} Z^2 \alpha^2 m_0 c^2 \qquad (25)$$

Let us arrange then (25) as follows

$$E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 \left[1 - (\sum_{p=1}^{q} \varepsilon_p)\right] \qquad (26)$$

As expressed, the second term of the right-hand side of equation (26) corresponds to the interaction energy of an electron-hydrogenic atom system of effective charge Z^* defined by

$$Z^{*2} = Z^2 \left[1 - (\sum_{p=1}^{q} \varepsilon_p)\right] \qquad (27)$$

Let us then put

$$\left[1 - \beta(1S_0, Z)\right]^2 = \left[1 - (\sum_{p=1}^{q} \varepsilon_p)\right] \qquad (28)$$

While using (28), the equations (26) and (27) are written respectively

$$W_1 = \varepsilon_1 Z^2 E_H \qquad (19)$$

For convenience of language, we will call ε_1 the perturbation coefficient taking into account the electron correlation to the first approximation. Using (14) and (19), let us write the value of the ground-state energy to the *p* orders of various approximation as follows:

$$E(1S_0) = -\frac{1}{2} Z^2 \alpha^2 m_0 c^2 - \frac{1}{2} Z^2 \alpha^2 m_0 c^2 \left[1 - \beta(1S_0, Z)\right]^2 \qquad (29)$$

$$Z^{*2} = Z^2 \left[1 - \beta(1S_0, Z)\right]^2 \qquad (30)$$

That is to say

$$Z^* = Z \left[1 - \beta(1S_0, Z)\right] \qquad (31)$$

As defined by (31), the $\beta(1S_0, Z)$-parameter plays the role of Screen Constant assumed to depend on the charge number *Z* and the number of electrons of the considered atomic system (two electrons in the case of helium isoelectronic sequence).

The result (31) gives the expression of the effective nuclear charge Z * to the ground state. This result is generalized to the case of doubly excited states $(N\ell, n\ell')$ $^{2S+1}L^\pi$ as follows:

$$Z^* = Z \left[1 - \beta(N\ell, n\ell', {}^{2S+1}L^\pi; Z)\right] \qquad (32)$$

$$E\left(1s^2\ {}^1S\right) = -Z^2\ Ryd - Z^2\left[1 - \beta(1S_0, Z)\right]^2 Ryd \quad (33)$$

In equation (33), the second term of the right-hand side gives the first ionization energy. As the lowest-energy

envelope ($N = 1$) contains the singly excited states series $(1s, n\ell')\ {}^{2S+1}L^\pi$ approaching the first ionization threshold, the total energy of the $(N\ell, n\ell')\ {}^{2S+1}L^\pi$ excited states with $n = N, N+1, N+2,...$ is expressed as follows:

$$E(N\ell, n\ell',\ {}^{2s+1}L^\pi) = -Z^2\left(\frac{1}{N^2} + \frac{1}{n^2}\left[1 - \beta(N\ell, n\ell',\ {}^{2s+1}L^\pi, Z)\right]^2\right) Ryd \quad (34)$$

In this equation, the main quantum numbers N and n and the orbital ℓ and ℓ' are performed respectively to the internal and external electron-electron, with the condition: n=N, N+1, N+2,…,. s respectively and L is the total spin and total angular momentum of the atomic system of the two π electrons and the parity of the considered quantum state and β is the Screen Constant by Unit Nuclear Charge. [19-22]

3. Results and Discussions

For all calculations, we fixed the value of $C_1 = 0.5$ and this choice has allowed us to have very good results comparable to other results and this will enable us in future to further reduce the terms of the wave function.

To calculate the energies, we used

For $2sns\ {}^{+1,3}S^e$ state: $C_2 = 4$ and the only parameter C_3 is varied.

For the $2snp\ {}^{+1,3}P^0$ and $2pnp\ {}^{+1,3}D^e$ states: $C_2 = 8$ and C_3 it is the only parameter which varied can explains through the increasing reduction of terms for the calculation of energy.

Table 1, 2, 3, 4 show the results of targeted energy $2s3s\ {}^{+1,3}S^e$, $2s4s\ {}^{+1,3}S^e$, $2s2p\ {}^{+1}P^0$, $2s2p\ {}^{+3}P^0$ $2s4p\ {}^{+1}P^0$, $2s2p\ {}^{+3}P^0$ $2s5p\ {}^{+1,3}P^0$, $2s6p\ {}^{+1,3}P^0$, and $2p3p\ {}^{+1,3}D^e$, $2p4p\ {}^{+1,3}D^e$ respectively. The calculations for each state take into consideration the Screen Constants α and deduce the value of the energy of the formula (34) for $2 \le Z \le 10$.

Table 1. Energy doubly excited $2sns\ {}^{+1,3}S^e$ states of He-like systems (Z=2-10). The energies E are in eV.

| | $2sns^{+1,3}S^e$ | | | | | | | | | | | |
| | $2s3s^{+1}S^e$ | | | $2s4s^{+1}S^e$ | | | $2s3s^{+3}S^e$ | | | $2s4s^{+3}S^e$ | | |
Z	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E
2	1.80	0.663459	16.306187	1.50	0.729604	14.978090	0.60	0.743241	15.993410	0.40	0.675160	15.098242
3	2.20	0.682478	38.732255	1.85	0.736960	34.967790	0.70	0.681944	38.736000	0.60	0.879856	34.435178
4	2.65	0.723437	70.652667	2.10	0.705284	63.653537	0.80	0.659242	71.294857	0.70	0.856291	62.826778
5	3.00	0.723104	112.688184	2.50	0.746761	100.418583	0.90	0.651543	113.621289	0.70	0.730257	100.538198
6	3.30	0.712025	164.723696	3.20	0.874885	144.787414	1.10	0.722112	164.562569	0.70	0.648290	146.806156
7	3.60	0.705430	226.567535	3.60	0.886240	198.454455	1.20	0.715839	226.369599	0.70	0.591638	201.591456
8	3.90	0.701023	298.229436	3.90	0.870421	260.915524	1.20	0.659631	299.145471	0.90	0.709733	262.885881
9	4.25	0.707015	379.483459	4.25	0.868153	331.746820	1.20	0.617393	381.742765	1.00	0.735745	333.592929
10	4.55	0.702858	470.812844	4.55	0.855679	411.248041	1.20	0.585029	474.145983	1.00	0.695791	413.756336

Table 2. Energy doubly excited $2snp\ {}^{+1}P^0$ states of He-like systems (Z=2-10). The energies E are in eV.

| | $2snp^{+1}P^0$ | | | | | | | | | | | |
| | $2s2p^{+1}P^0$ | | | $2s3p^{+1}P^0$ | | | $2s4p^{+1}P^0$ | | | $2s5p^{+1}P^0$ | | | $2s6p^{+1}P^0$ | | |
Z	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E
2	1.51	0.759983	18.894532	1.23	0.957725	15.247958	0.87	0.943334	14.555144	0.60	0.898891	14.265533	0.44	0.964665	14.010807
3	1.72	0.751725	47.810694	1.42	0.926908	37.109854	1.04	0.965049	34.134165	0.73	0.953702	32.891679	0.52	0.968484	32.172577
4	1.92	0.755942	90.318773	1.60	0.920405	68.760013	1.18	0.964131	62.260095	0.84	0.974109	59.405742	0.59	0.970758	57.890843
5	2.10	0.759537	146.474359	1.80	0.942207	109.927495	1.31	0.968935	98.853450	0.93	0.977237	93.842635	0.66	0.989045	91.115754
6	2.25	0.757718	215.925692	2.00	0.967647	160.735552	1.42	0.967884	143.984149	0.98	0.946715	136.348414	0.71	0.983270	131.963011
7	2.40	0.762678	299.123270	2.10	0.945497	222.085794	1.51	0.962342	197.668084	1.08	0.983581	186.369354	0.76	0.989981	180.320941
8	2.50	0.755721	396.187122	2.25	0.956707	292.685734	1.60	0.965728	259.767605	1.14	0.985718	244.467181	0.79	0.978708	236.322810
9	2.60	0.754630	506.673703	2.40	0.971378	372.960541	1.67	0.963922	330.430131	1.18	0.978716	310.5314170	0.82	0.977830	299.837474
10	2.70	0.757748	630.596387	2.50	0.970357	463.401665	1.73	0.963311	409.584014	1.22	0.979879	384.4221941	0.86	0.996218	370.780985

Table 3. *Energy doubly excited* $2snp^{+3}P^0$ *states of He-like systems (Z=2-10). The energies E are in eV.*

	$2snp^{+3}P^0$														
	$2s2p^{+3}P^0$			$2s3p^{+3}P^0$			$2s4p^{+3}P^0$			$2s5p^{+3}P^0$			$2s6p^{+3}P^0$		
Z	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E
2	3.44	0.556000	20.698117	3.30	0.784191	15.840338	2.75	0.834244	14.761311	2.20	0.893662	14.271819	1.69	0.949670	14.0226310
3	3.70	0.543556	51.137396	3.80	0.815060	37.829813	3.10	0.810237	34.690325	2.55	0.889757	33.036335	2.00	0.959599	32.186251
4	3.94	0.540040	95.142319	4.10	0.780880	70.088583	3.45	0.811769	63.066491	2.85	0.881215	59.716388	2.30	0.977198	57.876108
5	4.15	0.536875	152.790219	4.40	0.767597	112.115835	3.80	0.822573	99.875075	3.15	0.886487	94.244479	2.50	0.952296	91.227674
6	4.35	0.537093	223.961163	4.70	0.764260	163.892673	4.10	0.823648	145.236241	3.40	0.881699	136.708420	2.73	0.955958	132.066805
7	4.52	0.535400	308.818867	4.95	0.755740	225.613874	4.37	0.822325	199.122492	3.65	0.883812	187.028142	2.90	0.943668	180.532109
8	4.69	0.536837	407.146390	5.25	0.761597	296.898194	4.62	0.820815	261.519105	3.90	0.889846	245.204202	3.12	0.955589	236.445670
9	4.82	0.534572	519.273260	5.50	0.760416	378.148810	4.90	0.828138	332.301581	4.10	0.886850	311.338098	3.30	0.957940	299.958293
10	4.95	0.534659	644.885159	5.70	0.753804	469.384676	5.10	0.822671	411.762286	4.30	0.887265	385.336088	3.40	0.942656	371.146570

Table 4. *Energy doubly excited* $2pnp^{+1,3}D^e$ *states of He-like systems (Z=2-10). The energies E are in eV.*

	$2pnp^{+1,3}D^e$											
	$2p3p^{+1}D^e$			$2p4p^{+1}D^e$			$2p3p^{+3}D^e$			$2p4p^{+3}D^e$		
Z	C_3	α	-E	C_3	α	-E	C_3	α	-E	C_3	α	-E
2	0.80	0.804488	15.766353	0.50	0.621569	15.221433	2.69	0.794007	15.804405	2.30	0.976316	14.496810
3	0.93	0.811238	37.855101	0.65	0.795727	34.744544	2.98	0.753283	38.243704	2.40	0.803008	34.717296
4	1.10	0.876092	69.175602	0.70	0.756383	63.369428	3.30	0.755577	70.335827	2.80	0.858419	62.815407
5	1.30	0.959764	109.712571	0.90	0.938038	99.066087	3.55	0.744668	112.410046	3.20	0.905450	99.292115
6	1.40	0.952084	160.972715	1.00	0.969346	143.971650	3.80	0.743374	164.223971	3.50	0.914165	144.446344
7	1.50	0.955369	221.905240	1.05	0.953446	197.759513	4.02	0.740257	225.906559	3.70	0.897993	198.332373
8	1.60	0.965728	292.493746	1.10	0.949397	259.963213	4.25	0.743641	297.291657	3.90	0.889846	260.680306
9	1.70	0.981009	372.726899	1.08	0.895339	331.371468	4.45	0.743756	378.564276	4.20	0.909414	331.177628
10	1.75	0.973792	463.307924	1.20	0.964450	409.566509	4.65	0.746303	469.594466	4.20	0.866880	411.073951

Based on the processing of the calculations, energy conversion of 1 a.u. = 2Ry = 27.211385 eV was used. For the calculation of doubly excited states for Helium-like ions, several authors have used different methods. Thus, Ho [3, 23, 31] used the method of complex rotation convoluted with a wave function of Hylleraas type, Dieng [4] used Special Forms of Hylleraas-Type Wave Functions, Ivanov and Safronova [24] performed calculation using double sum method over the complete hydrogen spectrum, Sakho [25] with the Screening Constant by Unit Nuclear Charge method, Lipsky et al. [26], Ray and P. K. Mukherjee [27] with the time independent variation perturbation theory and Kar and Ho [28] the stabilization method, Drake and Dalgarno [29] the hydrogenic wave function for the continuum, Ho and A. Bathia [3] which have used the complex-coordinate rotation method.

In fact, a comparison is made in Table 5 based on the theoretical results from Ho [23], Dieng [4], Ivanov and Safronova [24], Sakho [25], Lipsky et al. [26], Ray and P. K. Mukherjee [27], Kar and Ho [28] for the $2s3s^{+1,3}S^e$, $2s4s^{+1,3}S^e$ states. For these state, best consistency of the results was found and a little discrepancies regard Dieng results.

Table 6 compares results with those from Ivanov and

Safronova [24], Ho [3, 23, 31], Drake and Dalgarno [29], Seminario and Sanders [30], Sakho [16, 32], Lipsky et al. [26], Ray and P. K. Mukherjee [27], Kar and Ho [28] for the $2s2p^{+1}P^0$, $2s3p^{+1}P^0$, $2s4p^{+1}P^0$ states. For these states, we note generally a quite good agreement.

In Table 7, results of $2s2p^{+3}P^0$, $2s3p^{+3}P^0$, $2s4p^{+3}P^0$ states were compared with those of Ho [23, 31], Sakho [25, 32], Drake and Dalgarno [29], Dieng [4], Seminario and Sanders [30], Lipsky et al. [28]. For these states, we note generally a quite good agreement and little discrepancy with Dieng results.

We have also compared in Table 8, results with those from Ho and A. Bathia [3], Dieng [4], Sakho [25], Lipsky et al. [26]. Ray and P. K. Mukherjee [27] for the $2p3p^{+1,3}D^e$, $2p4p^{+1,3}D^e$ states. We note good consistency.

In summary, we have calculated the singlet and triplet doubly excited states energies using a new wave function to four terms. We note here generally a satisfactory agreement between the present results and the other available calculations and we find a good agreement.

Table 5. *A comparison of the doubly excited* $2s3s$ $^{+1,3}S^e$, $2s4s$ $^{+1,3}S^e$ *states of He-like systems (Z = 2–10) with other results. The energies E are in eV.*

states		Z								
		2	3	4	5	6	7	8	9	10
	-Eᵖ	16.306187	38.732255	70.652667	112.688184	164.723696	226.567535	298.229436	379.483459	470.812844
	-Eᵃ	16.052676	38.519756	70.805384	112.913642	164.846570	226.602808	298.187799	379.596099	470.830431
	-Eᵇ	15.165734	37.115482	68.976266	110.800839	162.605813	224.396878	296.176160	377.944499	469.702254
$2s3s\,^1S^e$	-Eᶜ	16.063152	38.498395	70.769465	112.870924	164.800583	226.557638	298.141809	379.552556	470.790159
	-Eᵈ	16.643595	38.414137	70.658117	112.737602					
	-Eᵉ	16.196223	38.368068	70.350710	112.187143					
	-Eᶠ					164.845209		298.186166		470.829343
	-Eᵖ	14.978090	34.967790	63.653537	100.418583	144.787414	198.454455	260.915524	331.746820	411.248041
	-Eᵍ	14.566254	34.362536	62.662376	99.465774	144.772731	198.583244	260.897316	331.706782	411.027969
$2s4s\,^1S^e$	-Eᵇ	13.471787	32.829593	60.852820	97.598041	143.088282	197.333452	260.338149	332.104666	412.634221
	-Eᶜ	14.816599	34.722271	63.135039	100.052449	145.474511	199.400129	261.829854	332.763125	412.199963
	-Eᵈ	14.803516	33.661612	61.425971	100.102861					
	-Eᵉ	15.287362	35.159844	63.542419	100.445426					
	-Eᶠ					145.710436		262.171626		412.645959
	-Eᵖ	15.993410	38.736000	71.294857	113.621289	164.562569	226.369599	299.145471	381.742765	474.145983
	-Eᵍ	15.934986	38.414311	70.722389	112.856497	164.813916	226.600087	298.209567	379.653242	470.920228
$2s3s\,^3S^e$	-Eᵇ	16.095664	38.862656	71.581384	114.261149	162.605813	229.512933	302.086355	384.625137	477.129381
	-Eᶜ	16.367647	39.140856	71.761863	114.219787	166.508641	228.624613	300.571515	382.344449	473.943413
	-Eᵈ	15.219578	39.166559	71.781485	114.225276					
	-Eᵖ	15.098242	34.435178	62.826778	100.538198	146.806156	201.591456	262.885881	333.592929	413.756336
	-Eᵍ	14.726801	34.653697	63.084153	100.018166	145.455737	199.394144	261.838830	332.768026	412.225271
$2s4s\,^3S^e$	-Eᵇ	13.895917	33.726418	62.270834	99.540911	145.540779	200.272170	263.735914	335.932452	416.862037
	-Eᶜ	14.941770	34.982955	63.533141	100.592326	146.157790	200.224091	262.796671	333.882877	413.455225
	-Eᵈ	15.930095	34.082273	62.173822	100.636776					

ᵖ Present work, ᵃ Ho [23], ᵇ Dieng [4], ᶜ Sakho [25], ᵈ Lipsky [26], ᵉ Ray [27], ᶠ Kar [28], ᵍ Ivanov [24]

Table 6. *A comparison of the doubly excited* $2s2p$ $^{+1}P^0$, $2s3p$ $^{+1}P^0$, $2s4p$ $^{+1}P^0$ *states of He-like systems (Z = 2-10) with other results. All energies are given in eV.*

states		Z								
		2	3	4	5	6	7	8	9	10
	-Eᵖ	18.894532	47.810694	90.318773	146.474359	215.925692	299.123270	396.187122	506.673703	630.596387
	-Eᵃ	18.861170	47.825661	90.327684	146.403024	216.066103	299.324403	396.181326	506.640138	630.699613
$2s2p\,^1P^0$	-Eᶜ	18.894913	47.772871	90.283874	146.341799	216.095763	299.410255	396.330445	506.856332	630.987918
	-Eʰ	18.872191	47.827565	90.345916	146.422617	216.086511	299.345220	396.202551	506.660683	630.720974
	-Eᴵ	18.844980	47.810694	90.311630	146.385881	216.048143	299.305491	396.161734	506.618233	630.677708
	-Eᵖ	15.247958	37.109854	68.760013	109.927495	160.735552	222.085794	292.685734	372.960541	463.401665
	-Eᵃ	15.347221	37.046396	68.525070	109.807462	160.905001	221.820407	292.557763	373.119789	463.503766
$2s3p\,^1P^0$	-Eᶜ	15.303409	37.026531	68.578132	109.951546	161.153712	222.182046	293.036819	373.717759	464.225139
	-Eᵈ	15.317839	36.913428	68.270671	109.449241					
	-Eᶠ					160.905736		292.559804		463.505807
	-Eᵖ	14.555144	34.134165	62.260095	98.853450	143.984149	197.668084	259.767605	330.430131	409.584014
	-Eᵃ	14.540703								
$2s4p\,^1P^0$	-Eᶜ	14.522852	34.146478	62.273797	98.904676	144.039111	197.677106	259.818521	330.463630	409.612297
	-Eᵈ	14.527211	34.090328	62.146447	98.651052					
	-Eᶠ					144.012445		259.751963		409.503044

ᵖ Present work, ᵃ Ho [31] for 2s2p state, ᵃ Ho [23] for 2s3p state, ᵃ Ho [3] for 2s4p state, ᶜ Sakho [32] for 2s3p state,
ᶜ Sakho [24] for 2s2p and 2s4p states, ᵈ Lipsky [26], ᵉ Ray [27], ᶠ Kar [28], ᵍ Ivanov [24], ʰ Drake [29], ᴵ Seminario [30]

Table 7. *A comparison of the doubly excited $2s2p\ ^{+3}P^0$, $2s3p\ ^{+3}P^0$, $2s4p\ ^{+3}P^0$ states of He-like systems (Z = 2–10) with other results. All energies are given in eV.*

states		Z								
		2	3	4	5	6	7	8	9	10
$2s2p^3P^0$	$-E^P$	20.698117	51.137396	95.142319	152.790219	223.961163	308.818867	407.146390	519.273260	644.885159
	$-E^a$	20.694130	51.108035	95.121108	152.737293	223.957544	308.782812	407.158812	519.248946	644.890084
	$-E^c$	20.784744	51.076606	94.974030	152.477152	223.585972	308.300490	406.620706	518.546620	644.078232
	$-E^h$	20.696171	51.109804	95.122876	152.738926	223.959177	308.784309	407.214731	519.250443	644.891309
	$-E^I$	20.720661	51.140689	95.157027	152.774981	223.996728	308.822813	407.253915	519.289355	644.889676
$2s3p^3P^0$	$-E^P$	15.840338	37.829813	70.088583	112.115835	163.892673	225.613874	296.898194	378.148810	469.384676
	$-E^a$	15.756208	38.055503	70.185101	112.141383	163.923832	225.532448	296.967232	378.228224	469.315437
	$-E^b$	15.639786	37.778908	69.638936	111.275300	162.754336	224.161617	295.608303	377.239537	469.247677
	$-E^c$	15.945580	38.226553	70.333538	112.266826	164.026554	225.612449	298.874886	378.263421	469.335178
	$-E^d$	15.873876	38.176280	70.323335	112.310764					
$2s4p^3P^0$	$-E^P$	14.761311	34.690325	63.066491	99.875075	145.236241	199.122492	261.519105	332.301581	411.762286
	$-E^a$	14.771353								
	$-E^b$	13.708117	33.264523	61.414127	98.168803	143.532748	197.507757	260.094734	331.294203	411.106516
	$-E^c$	14.785578	34.646486	63.010954	99.878979	145.250563	199.125703	261.504402	332.386658	411.772473
	$-E^d$	14.754046	34.629494	63.019035	99.274383					

[p] Present work, [a] Ho [31], [a] Ho [23] for 2s3p state, [a] Ho [3] for 2s4p state, [b] Dieng [4], [c] Sakho [32] for 2s3p state and
[c] Sakho [25] for 2s4p state, [d] Lipsky [28], [e] Ray [27], [f] Kar [28], [g] Ivanov [24], [h] Drake [29], [I] Seminario [30]

Table 8. *A comparison of the doubly excited $2p3p\ ^{+1,3}D^e$, $2p4p\ ^{+1,3}D^e$ states of He-like systems (Z = 2–10) with other results. All energies are given in eV.*

states		Z								
		2	3	4	5	6	7	8	9	10
$2p3p^1D^e$	$-E^P$	15.766353	37.855101	69.175602	109.712571	160.972715	221.905240	292.493746	372.726899	463.307924
	$-E^a$		36.631163	67.882894	108.926902	159.777905	220.443374	290.927393	371.232543	461.360052
	$-E^b$	14.913710	36.509663	67.865484	109.033816	160.030974	220.862438	291.530211	372.035049	462.377265
	$-E^c$	15.485182	37.385721	69.114741	110.670875	162.053864	223.263429	294.299849	375.162008	465.851021
	$-E^d$	15.132719	36.575789	67.756894	108.731894					
	$-E^e$	15.888735	37.557169	69.041842	110.369422					
$2p4p^1D^e$	$-E^P$	15.221433	34.744544	63.369428	99.066087	143.971650	197.759513	259.963213	331.371468	409.566509
	$-E^b$	13.278352	32.357248	59.195913	96.195913	141.035323	194.505733	256.611737	327.355621	406.738598
	$-E^c$	14.597547	34.295053	62.496931	99.202368	144.411631	198.124729	260.341114	331.061326	410.285104
	$-E^d$	14.402121	33.890895	61.866605	98.436218					
	$-E^e$	15.164911	34.825144	63.006354	99.707997					
$2p3p^3D^e$	$-E^P$	15.804405	38.243704	70.335827	112.410046	164.223971	225.906559	297.291657	378.564276	469.594466
	$-E^a$	15.885578	38.247460	70.432249	112.441374	164.274947	225.934290	297.419419	378.730498	469.867643
	$-E^b$	15.822041	38.203796	70.372148	112.336311	164.098917	225.660899	297.022644	378.184333	469.146057
	$-E^c$	15.874305	38.191995	70.352586	112.346014	164.169003	225.820208	297.298799	378.604517	469.737080
	$-E^d$	15.869550	38.204963	70.368588	112.362194					
$2p4p^3D^e$	$-E^P$	14.496810	34.717296	62.815407	99.292115	144.446344	198.332373	260.680306	331.177628	411.073951
	$-E^b$	13.708141	33.264567	61.414168	98.168776	143.532539	197.507189	260.093552	331.292066	411.102982
	$-E^c$	14.714556	34.576691	62.954899	99.841564	145.234241	199.13209	261.534064	332.443919	411.850573
	$-E^d$	14.402692	33.897889	61.899667	99.802039					

[p] Present work.
[a] Ho and A. Bathia [3]
[b] Dieng [4]
[c] Sakho [25],
[d] Lipsky [26]
[e] Ray [27]

4. Conclusion

The method of Hylleraas was successfully applied by himself in the calculation of the energy of the ground state of helium and its isoelectronic series.

To expand this application to calculate the total energy of atomic systems in the doubly excited states we used a new wave function correlated with four terms adapted to the description of these conditions and using the method of Screen Constant by Unit Nuclear Charge, which has the advantage of leading to very accurate results as was the case in several approximation methods applied to the treatment of the properties of atomic systems with two electrons. [33-34]

It has been demonstrated the possibilities to use the screening constant by unit nuclear charge method in the study of $2sns^{+1,3}S^e$, $2snp^{+1,3}P^0$ and $2pnp^{+1,3}D^e$ doubly excited states in the helium-like ions in the framework of a variational procedure. Thus, a new correlated wave function is performed and results obtained are shown by the comparison with various available theoretical literature values (See Table 5-8). 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.

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