



# Correlation Factor Taking into Account Spherical Harmonics Through Hypergeometric Functions to Calculate Energies of Li-Like Ions

Boubacar Sow<sup>\*</sup>, Malick Sow, Ahmadou Wagué

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

## Email address:

boubacar1.sow@ucad.edu.sn (B. Sow)

<sup>\*</sup>Corresponding author

## To cite this article:

Boubacar Sow, Malick Sow, Ahmadou Wagué. Correlation Factor Taking into Account Spherical Harmonics Through Hypergeometric Functions to Calculate Energies of Li-Like Ions. *International Journal of Applied Mathematics and Theoretical Physics*.

Vol. 6, No. 2, 2020, pp. 26-34. doi: 10.11648/j.ijamtp.20200602.13

**Received:** May 6, 2020; **Accepted:** July 14, 2020; **Published:** July 28, 2020

---

**Abstract:** Calculations of the energy levels of atoms and ions with  $Z \leq 10$  are carried out in this paper using a new wave function including a new method to calculate the correlation factor taking into account spherical harmonics through hypergeometric functions to calculate  $(1s22s) \ ^2S^e$ ,  $(1s2s) \ ^2S^e$ ,  $(1s2sns) \ ^2S^e$  and  $(1s2snp) \ ^2P^o$  states. The calculations concern the total energy, kinetic energy, Coulomb interaction between the atomic nucleus and the three electrons and the Coulomb interaction between electrons. The results that we have obtained confirm that a relatively theoretical procedure could be used for adequate calculations and understanding of electron correlation effects in doubly excited three- electron states. These results are in compliance with some experimental and theoretical data.

**Keywords:** Wave Function Correlated, Spherical Harmonics, Excited States, Correlation Factor

---

## 1. Introduction

In recent years, the importance of electron-electron interaction has been widely recognized during multi-excitation and multi-ionization processes. The study of doubly excited He-like systems (ideal for tackling the Coulomb problem with three bodies) made it possible to clarify the theoretical discussions related to the energy position of excited levels and to check the reliability of multi-configuration type calculations [1-4]. Systems with three excited electrons (four-body Coulomb problem) are more difficult to deal with. The study of states with three excited electrons, first carried out on the He- ion after diffusion of electrons on helium atoms [5], made it possible to observe the  $(2s^22p) \ ^2P^o$  and  $(2s2p^2) \ ^2D^e$  identified at 1 using the theoretical results of Fano and Cooper [6]. Subsequently, it was easier to start from the lithium atom (with three electrons) than to previously capture an electron on He [7, 8]. In addition, the lithium atom constitutes an excellent system for study the four-body Coulomb problem. With this atom, the accent was put on the creation of hollow ionic states by ionization-

excitation in layer K [6, 9-11]. Likewise, the effect of the term  $1 / r_{ij}$ , which describes the electrostatic repulsion between the electrons, is very important: Consider for example the case of the Helium atom. If we neglect it, we find for the fundamental level an energy of -108.8 eV (2 electrons subjected to  $Z=2$ ) instead of -79eV for the experimental value (corresponding to the energy of double ionization of this atom). This same calculation leads to an energy value of simple ionization of the atom of 54.4 eV to compare with the experimental value of 24.6 eV. We must therefore take this term into account. It's for this reason we have chosen a wave function of lesser terms which mainly takes into account this interaction. According to the calculations, we see that: the radial correlation expectation values  $1/r_{ij}$  of three electron systems increase when  $Z$  increases, as is the case for two electron systems [12-15]. The ratios and the differences with respect to the results of Uptal and Talukdar [12] are practically constants. And for the same atomic systems,  $1/r_{12}$  in the lithium-like ions (3.44 Rydbergs in the case of Li for example) is greater than that of the corresponding helium-like ions (3.2 Rydbergs for  $Li^+$ ). This

result indicates that the two electrons in the  $1s^2 2S^e$  closed shell core are closer to each other compared to the two electrons in the corresponding helium isoelectronic series. This points out that, in the ground state, the electron-electron effects due to the third electron, decreases the probability of the two electrons in the  $1s^2 2S^e$  closed shell core to go far away, and far away from each other, when increasing the charge number  $Z$ .

## 2. Wave Functions and Calculations

Schrödinger equation for the Li-like atom and its isoelectronic series attracted a considerable amount of effort.

Lithium isoelectronic sequence serve as prototypes for alkali metal atoms and alkaline earth cations [16]. They are a good test for ab-initio calculation methods. Similarly, Hylleraas-type wave functions containing  $r_{ij}$  factors have been widely used in

atomic physics to study the correlation effects between electrons and / or between electrons and the nucleus for bound and scattering states [17]. The first calculations on the fundamental state of lithium were made by Eckart [18], Guillemin and Zener [19], Wilson [20], and James and Coolidge [21, 22].

Since then, the ground state energy of Lithium has been carried out by Weiss [23], Muszynska et al. [24], King et al. [25-27], McKenzie and Drake [28], Luchow and Kleindienst [29], and Yan et al. [30, 31]. All these studies, except that of Weiss [23], use Hylleraas-type wave functions, of several terms ranging from 100 terms [32] to 3502 terms [31]. The use of Hylleraas-type wave functions have led to fairly precise results in various branches of atomic physics. The new special wave functions containing fewer terms used in this work is defined by:

$$\psi(j, k, m, j', k', m') = \left\{ \sum_{\gamma=0}^{N-L-1} (N^2 r_0^2 L)^\gamma \sum_{\nu=0}^{n_3-\ell_3-1} (n_3^2 r_0^2 \ell_3)^\nu (C_{jkm} + C_{j'k'm'}) \right\} x(r_{12}^J r_{13}^K r_{23}^M) e^{-(\alpha_1 r_1 + \alpha_2 r_2 + \alpha_3 r_3)} \quad (1)$$

Where  $J+K+M \leq \Omega$ ,  $\Omega$  is a positive integer number which determines the expansion length  $N$ ;  $\alpha_1, \alpha_2, \alpha_3$  are a nonlinear parameter  $r_1, r_2$  and  $r_3$  are the coordinates of electrons with respect to the nucleus,  $\ell_1, \ell_2, \ell_3$  are respectively the orbital angular moments of the three electrons.  $C_{jkm}$  and  $C_{j'k'm'}$  are parameters to be determined,  $r_0$  is Bohr radius.  $L = \ell_1 + \ell_2$ ,

$N = n_1 + n_2$ .  $J = j + j'$ ,  $K = k + k'$  and  $M = m + m'$ . The resonance parameters are determined by finding a rate of change which is stable with respect for the non-linear parameters  $\alpha_1, \alpha_2, \alpha_3$ . According to the calculation of correlation coefficients, proposed by Varshalovich D. A et al. [33], we found a new formula that is proposed by Gning et al. [34]:

$$r_{ij}^q = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} a_\ell^q(r_i, r_j) \times (Y_{\ell, m_i}(\Omega_1) Y_{\ell, m_j}(\Omega_2)) \quad \text{For } r_i < r_j \quad (2)$$

With

$$a_\ell^q(r_i, r_j) = \frac{\left(\frac{-q}{2}\right)_\ell}{\left(\frac{1}{2}\right)_\ell} r_j^q \left(\frac{r_i}{r_j}\right)^\ell F\left(\ell - \frac{q}{2}, -\frac{1}{2} - \frac{q}{2}, \ell + \frac{3}{2}, \frac{r_i^2}{r_j^2}\right) \quad (3)$$

The hypergeometric wave function defined by Samarskogo [35]

$$F\left(\ell - \frac{q}{2}, -\frac{1}{2} - \frac{q}{2}, \ell + \frac{3}{2}, \frac{r_i^2}{r_j^2}\right) = 1 - \frac{(2\ell - q)(1 + q)}{2(2\ell + 3)} \times \frac{r_i^2}{r_j^2} \quad (4)$$

Replacing equation (4) with its value in equation (3)

$$a_\ell^q(r_i, r_j) = \frac{\left(\frac{-q}{2}\right)_\ell}{\left(\frac{1}{2}\right)_\ell} r_j^q \left(\frac{r_i}{r_j}\right)^\ell \times \left(1 - \frac{(2\ell - q)(1 + q)}{2(2\ell + 3)} \times \frac{r_i^2}{r_j^2}\right) \quad (5)$$

So equation (5) becomes

$$a_\ell^q(r_i, r_j) = \frac{\left(\frac{-q}{2}\right)_\ell}{\left(\frac{1}{2}\right)_\ell} \times \frac{r_i^\ell}{r_j^{\ell-q+2}} \times (r_j^2 - \frac{(2\ell - q)(1 + q)}{2(2\ell + 3)} \times r_i^2) \quad (6)$$

And replacing equation (6) in equation (2)

$$r_{ij}^q = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \times \frac{\left(\frac{-q}{2}\right)_{\ell}}{\left(\frac{1}{2}\right)_{\ell}} \times \frac{r_i^{\ell}}{r_j^{\ell-q+2}} \times \left[ r_j^2 - \frac{(2\ell-q)(1+q)}{2(2\ell+3)} \times r_i^2 \right] \times (Y_{\ell_i, m_i}(\Omega_i) Y_{\ell_j, m_j}(\Omega_j)) \tag{7}$$

We obtain:

$$r_{12}^J = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \frac{\left(\frac{-J}{2}\right)_{\ell}}{\left(\frac{1}{2}\right)_{\ell}} \times \frac{r_1^{\ell}}{r_2^{\ell-J+2}} \times \left[ r_2^2 - \frac{(2\ell-J)(1+J)}{2(2\ell+3)} \times r_1^2 \right] \times (Y_{\ell_1, m_1}(\Omega_1) Y_{\ell_2, m_2}(\Omega_2)) \tag{8}$$

$$r_{13}^K = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \frac{\left(\frac{-K}{2}\right)_{\ell}}{\left(\frac{1}{2}\right)_{\ell}} \times \frac{r_3^{\ell}}{r_1^{\ell-K+2}} \times \left[ r_1^2 - \frac{(2\ell-K)(1+K)}{2(2\ell+3)} \times r_3^2 \right] \times (Y_{\ell_1, m_1}(\Omega_1) Y_{\ell_3, m_3}(\Omega_3)) \tag{9}$$

$$r_{23}^M = 4\pi \sum_{\ell=0}^{\infty} \frac{1}{2\ell+1} \frac{\left(\frac{-M}{2}\right)_{\ell}}{\left(\frac{1}{2}\right)_{\ell}} \times \frac{r_2^{\ell}}{r_3^{\ell-M+2}} \times \left[ r_3^2 - \frac{(2\ell-M)(1+M)}{2(2\ell+3)} \times r_2^2 \right] \times (Y_{\ell_2, m_2}(\Omega_2) Y_{\ell_3, m_3}(\Omega_3)) \tag{10}$$

Where

$$Y_{\ell_i, m_i}(\Omega_i) Y_{\ell_j, m_j}(\Omega_j) = \sum_{m=-\ell}^{\ell} Y_{\ell_i, m_i}^*(\Omega_i) Y_{\ell_j, m_j}(\Omega_j) \tag{11}$$

represent the spherical harmonics of electron i or j.

Which  $\Omega_i = (\theta_i, \varphi_i)$ ,  $\Omega_j = (\theta_j, \varphi_j)$  and  $i, j=1, 2, 3$ . For a given angular momentum  $L$ , the angular coupling for the three electrons is:  $(\ell_1, \ell_2, \ell_3)=(0, 0, 0)_A$  for S states and

$$Y_{0,0}(\Omega_i) Y_{0,0}(\Omega_j) = \frac{1}{4\pi} \tag{12}$$

$(\ell_1, \ell_2, \ell_3)=(0, 0, 1)_A (0, 1, 0)_B$  for P states,

$$Y_{\ell}(\Omega_i) Y_{\ell}(\Omega_j) = Y_{1,-1}^*(\Omega_i) Y_{1,-1}(\Omega_j) + Y_{1,0}^*(\Omega_i) Y_{1,0}(\Omega_j) + Y_{1,1}^*(\Omega_i) Y_{1,1}(\Omega_j) \tag{13}$$

by replacing the values of the spherical harmonics of e- i or j, we obtain:

$$Y_{\ell}(\Omega_i) Y_{\ell}(\Omega_j) = \frac{3}{4\pi} \begin{pmatrix} \sin \theta_i \sin \theta_j \cos \varphi_{ij} \\ + \cos \theta_i \cos \theta_j \end{pmatrix} \tag{14}$$

For  $\varphi_i = \varphi_j$  we have  $\cos \varphi_{ij}=1$

$$Y_{\ell}(\Omega_i) Y_{\ell}(\Omega_j) = \frac{3}{4\pi} (\sin \theta_i \sin \theta_j + \cos \theta_i \cos \theta_j) \tag{15}$$

$(\ell_1, \ell_2, \ell_3)=(0, 0, 2)_A (0, 1, 1)_B$  for D states,

$$Y_{\ell}(\Omega_i) Y_{\ell}(\Omega_j) = \sum_{m=-\ell}^{\ell} Y_{\ell, m}^*(\Omega_i) Y_{\ell, m}(\Omega_j) = \frac{15 \sin^2 \theta_i \sin^2 \theta_j}{16\pi} - \frac{15 \cos \theta_i \sin \theta_i \sin \theta_j^2}{8\pi} - \frac{\sqrt{75} (3 \cos^2 \theta_i - 1) \sin \theta_j^2}{2^{9/2} \pi} \tag{16}$$

The non-relativistic Hamiltonian complex of three-electron atomic systems is written in the form (in atomic units):

$$\hat{H} = -\frac{1}{2} \sum_{i=1}^3 \Delta_i - Z \sum_{i=1}^3 \left( \frac{1}{r_i} \right) + \sum_{\substack{i,j=1 \\ i < j}}^3 \left( \frac{1}{r_{ij}} \right) = T + C + W \quad (17)$$

In equation (17),  $T$  is the kinetic energy;  $C$  is the Coulomb interaction between the atomic nucleus and the two electrons and  $W$  is the Coulomb interaction between electrons. Where the Laplacian is written in the form:

$$\Delta_i = \frac{1}{r_i^2} \frac{\partial}{\partial r_i} \left( r_i^2 \frac{\partial}{\partial r_i} \right) + \frac{1}{r_i^2 \sin \theta_i} \frac{\partial}{\partial \theta_i} \left( \sin \theta_i \frac{\partial}{\partial \theta_i} \right) + \frac{1}{r_i^2 \sin^2 \theta_i} \frac{\partial^2}{\partial \varphi_i^2} = \Delta_{r_i} + \Delta_{\theta_i} + \Delta_{\varphi_i} \quad (18)$$

$$\begin{cases} \Delta_{r_i} = \frac{1}{r_i^2} \frac{\partial}{\partial r_i} \left( r_i^2 \frac{\partial}{\partial r_i} \right) \\ \Delta_{\theta_i} = \frac{1}{r_i^2 \sin \theta_i} \frac{\partial}{\partial \theta_i} \left( \sin \theta_i \frac{\partial}{\partial \theta_i} \right) \\ \Delta_{\varphi_i} = \frac{1}{r_i^2 \sin^2 \theta_i} \frac{\partial^2}{\partial \varphi_i^2} \end{cases} \quad (19)$$

With

$$\begin{aligned} T &= -\frac{1}{2} (\Delta_1 + \Delta_2 + \Delta_3) \\ &= -\frac{1}{2} \langle \psi^* (j, k, m, j', k', m') | (\Delta_1 + \Delta_2 + \Delta_3) | \psi (j, k, m, j', k', m') \rangle \end{aligned} \quad (20)$$

$$\begin{aligned} C &= -Z \left( \frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} \right) \\ &= -Z \langle \psi^* (j, k, m, j', k', m') | \frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} | \psi (j, k, m, j', k', m') \rangle \\ &= -Z \iiint dr_1^3 dr_2^3 dr_3^3 \psi^* (j, k, m, j', k', m') \left( \frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} \right) \psi (j, k, m, j', k', m') \end{aligned} \quad (21)$$

$$\begin{aligned} W &= \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \\ &= \langle \psi^* (j, k, m, j', k', m') | \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) | \psi (j, k, m, j', k', m') \rangle \\ &= \iiint dr_1^3 dr_2^3 dr_3^3 \psi^* (j, k, m, j', k', m') \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \psi (j, k, m, j', k', m') \end{aligned} \quad (22)$$

The normalization constant:

$$N_{j,k,m,j',k',m'} = \langle \psi (j, k, m, j', k', m') | \psi (j, k, m, j', k', m') \rangle \quad (23)$$

$$N_{j,k,m,j',k',m'} = \iiint dr_1^3 dr_2^3 dr_3^3 \Psi_{j,k,m,j',k',m'}^* \times \Psi_{j,k,m,j',k',m'} \quad (24)$$

With

$$\iiint dr_i^3 = \int_0^\infty dr_i \int_0^\pi d\theta_i \int_0^{2\pi} d\phi_i r_i^2 \sin \theta_i \quad (25)$$

and  $i=1, 2, 3$ .

### 3. Results and Discussions

In our calculations, we set the dimension  $\Omega$  to 4 for the  $(1s^2 2s) \ ^2S^e$  and  $(1s^2 2p) \ ^2P^0$  states and  $\alpha_1=\alpha_2=4.255$ ,  $\alpha_3=5.400$   $\Omega=3$  for the  $1s3s^2$ ,  $1s4s^2$  states and  $\alpha_1=6.754$ ,  $\alpha_2=7.350$ ,  $\alpha_3=5.403$ . Similarly  $\alpha_1=0.25$  for the  $(1s2sns) \ ^2S^e$  states and  $\Omega=4$  for the  $(1s2snp) \ ^2P^0$   $\alpha_1=\alpha_2=\alpha_3=2.600$ .  $\Omega=3$  for the  $(1s2sns) \ ^2S^e$  and  $(1s2snp) \ ^2P^0$  ( $n \leq 3$ ) and  $\alpha_1=4.250$ ,  $\alpha_2=8.550$ ,  $\alpha_3=7.855$ . After having fixed these parameters, we have Based on the processing of the calculations and energy conversion of 1 a. u.=2Ry=27.211385 eV was used.

Table 1 lists and compare our results for the  $(1s^2 2s) \ ^2S^e$  and  $(1s^2 2p) \ ^2P^0$  states of the lithium-like ions compared to the Hylleraas results (HR), the multiconfiguration Hartree-Fock (MCHF) and configuration interaction (CI).

The lithium ground-state isoelectronic sequence was investigated Perkins [36], and by Ho [17] using Hylleraas coordinates and calculations on the lithium isoelectronic sequences for some low-lying excited  $S$  states were carried out by King [37-38].

Chung, Zhu, and Wang [14] calculated isoelectronic sequences for some low-lying excited states using a full core plus correlation (FCPC) method. And I. sakho [46] using Screening Constant by Unit Nuclear Charge (SCUNC). Regarding the total energy, comparison shows that our results

agree well with all auteurs.

Table 2, Table 3, Table 4 show the results of targeted energy  $(1sns^2) \ ^2S^e$ ,  $(1s2sns) \ ^2S^e$ ,  $(1s2snp) \ ^2P^0$ . All result shows the relatively good accuracy obtained for the values of the energies of atomic systems studied in this work. We can notice that the kinetic energy  $T$  and the correlation energy between the two electrons  $W$  increase with the nuclear charge number  $Z$ , and decrease when the principal quantum number  $n$  increases.

These results point out that the electron correlation effects in the doubly excited states induce the decrease of the probability of electrons to be near the nucleus, as mentioned by Arias de Saavedra et al. [39].

Comparisons of our results concerning the total and excitation energies of the  $(1s2sns) \ ^2S^e$  and  $(1s2snp) \ ^2P^0$  ( $n \leq 3$ ) levels of Li-like ions ( $Z \leq 6$ ) with other theoretical values [14] and experimental data [40, 15] are given in Tables 5. Regarding the comparison with the results of Bhatia [14] listed in Table 5, the ratios between the present total energy calculation ( $E^a$ ) and that of Bhatia [14] ( $E^b$ ) are practically constants and equal to  $E^a/E^b \approx 1.00$ . This may indicate the good agreement between the present calculation and the quasiprojection operator results of Bhatia.

In the same way, considering the results quoted in Table 6, it is seen that the energy ratios between the present calculation and that of Erkoç and Jansen [40] and of David and Chung [15] are practically constant and respectively equal to  $E^c/E^d \approx 1$ .

These ratios point out the good agreement between our results and that of Erkoç and Jansen [40] using a density functional theory and that of David and Chung [15] employing the complex rotation method. Therefore, it should be mentioned that our results are most close to the density functional results of Erkoç and Jansen [40].

**Table 1.** Comparison of our results in the calculation of total energy of the  $(1s^2 2s) \ ^2S^e$  and  $(1s^2 2p) \ ^2P^0$  doubly excited states in the lithium-like ions. The energies are expressed in Rydbergs.

Author	Method	Ref	-E $(1s^2 2s) \ ^2S^e$	-E $(1s^2 2p) \ ^2P^0$
		Li		
Present work			14.955490	14.8204196
Chung and Zhu	FCPC	[42]	14.956119	14.8203156
Pipin and Bishop	CI-HR	[43]	14.956120	14.8203108
Tong et al.	MCHF	[44]	14.956121	14.8203062
Yan and Drake	HR	[41]	14.956120	14.8203130
Pestka and Woznicki	CI-HR	[45]	14.9561202	14.8203118
		Be <sup>+</sup>		
Present work			28.650490	28.357542
Chung and Zhu	FCPC	[42]	28.649522	28.358664
I. sakho	SCUNC	[46]	28.650495	29.273420
Perkins	HR	[36]	28.649140	
Ho	HR	[17]	28.649392	
King	HR	[37]	28.649520	
		B <sup>2+</sup>		
Present work			46.85536	46.56737
Chung and Zhu	FCPC	[42]	46.84920	46.40888
I. sakho	SCUNC	[46]	46.85548	64.29986
Perkins	HR	[36]	46.84872	
Ho	HR	[17]	46.84904	
		C <sup>3+</sup>		
Present work			69.56203	68.9620343
Chung and Zhu	FCPC	[42]	69.55101	68.9641964
Perkins	HR	[36]	69.55044	

Author	Method	Ref	-E (1s <sup>2</sup> 2s) <sup>2</sup> S <sup>e</sup>	-E (1s <sup>2</sup> 2p) <sup>2</sup> P <sup>o</sup>
I. sakho	SCUNC	[46]	69.56245	
Ho	HR	[17]	69.550836	
		N <sup>4+</sup>		
Present work			96.76975	96.026472
Chung and Zhu	FCPC	[42]	96.75378	96.022096
Perkins	HR	[36]	96.75314	
I. sakho	SCUNC	[46]	96.76951	
Ho	HR	[17]	96.75359	
		O <sup>5+</sup>		
Present work			128.476310	127.586316
Chung and Zhu	FCPC	[42]	128.457077	127.581463
Perkins	HR	[36]	128.45638	
I. sakho	SCUNC	[46]	128.476180	
Ho	HR	[17]	128.456870	
		F <sup>6+</sup>		
Present work			164.68247	162.9982479
Chung and Zhu	FCPC	[42]	164.66066	163.6417488
King	HR	[38]	164.660672	
		N <sub>e</sub> <sup>7+</sup>		
Present work			205.3882100	203.7658217
Chung and Zhu	FCPC	[42]	205.3644556	204.2026316
I. sakho	SCUNC	[46]	205.3881396	
King	HR	[38]	205.364458	

**Table 2.** Total energy and excitation energy of the (1sns<sup>2</sup>) <sup>2</sup>S<sup>e</sup> doubly excited states of three electron systems up to Z=10 (in Ryd). The excitation energies are calculated with respect to the ground state of the corresponding system.

Z	-E							
	3	4	5	6	7	8	9	10
(1sns <sup>2</sup> ) <sup>2</sup> S <sup>e</sup>								
1s2s <sup>2</sup>	10.8104	20.0884	32.4401	48.0874	66.5243	87.9402	112.5540	139.7926
1s3s <sup>2</sup>	9.8031	17.8987	28.2989	41.3667	55.7858	74.5286	93.87265	118.4367
1s4s <sup>2</sup>	8.9504	17.0544	26.9076	38.0735	53.3674	68.9687	88.8221	109.9467

**Table 3.** Total energies of (1s2sns) <sup>2</sup>S<sup>e</sup> doubly excited states in the Li-like ions. The energies are expressed in rydbergs.

Z	-E							
	3	4	5	6	7	8	9	10
ns								
2s	10.7973	19.8935	32.4376	48.0376	67.02571	87.3235	112.9873	139.0435
3s	10.3188	18.5437	32.4517	44.7643	61.6572	81.2256	102.9876	128.0236
4s	10.0092	18.3457	29.7732	43.5297	59.9273	78.9217	100.6759	124.9876
5s	10.0588	18.0281	27.4857	40.3275	57.2329	76.8892	99.3456	122.9843
6s	10.2201	18.2854	30.2046	42.4675	57.4578	75.7683	97.5678	122.6753
7s	10.8546	17.9876	29.0276	41.4597	59.7654	76.9745	97.4567	120.8796
8s	9.98745	16.5498	28.9764	42.3287	58.2345	77.0897	97.3476	119.7654
9s	9.9586	18.3457	29.0146	42.3234	58.9876	76.0345	97.0237	119.4357
10s	9.9545	18.2904	26.9875	42.0987	58.0675	76.4216	96.4568	119.0345

**Table 4.** Total energies of (1s2snp) <sup>2</sup>P<sup>o</sup> doubly excited states in the Li-like ions. The energies are expressed in rydbergs.

Z	-E							
	3	4	5	6	7	8	9	10
np								
2p	10.5687	19.7765	33.0987	45.7895	65.8976	86.9243	111.1765	138.3476
3p	10.3245	19.2098	31.8765	44.0987	62.7658	82.0985	107.4877	134.5568
4p	10.2457	18.9987	30.0756	43.4908	60.3452	79.0983	102.4758	127.8764
5p	10.1945	18.5432	29.7457	43.2357	59.8796	78.7895	101.8763	123.7543
6p	10.0087	18.3476	29.4356	43.1765	59.5678	78.2187	100.0245	122.9876
7p	9.9876	18.1298	29.3457	43.0547	59.3298	77.7865	99.3457	122.5678
8p	9.7843	18.0325	29.1045	42.9754	59.1204	77.3495	98.7568	122.3457
9p	9.6543	17.9876	29.10134	42.5467	58.9873	77.2175	98.2963	122.0453
10p	9.5432	17.7463	28.9457	42.3457	58.7595	77.05473	98.1134	121.8769

**Table 5.** Comparison of our results in the calculation of total energy of the  $(1s2sns)^2S^e$  and  $(1s2snp)^2P^o$  ( $n \leq 3$ ) doubly excited states in the lithium-like ions ( $Z \leq 6$ ). The energies are expressed in Rydbergs.

Systeme	$(1s2snl)^2L^{\pi}$	Present work	Bathia	Rapport <sup>a</sup> E <sup>a</sup> /E <sup>P</sup>
		$-E (1s2snl)^2L^{\pi}$	$-E (1s2snl)^2L^{\pi}$	
Li	$(1s2s2s)^2S^e$	10.7973	10.8090	1.001083
	$(1s2s3s)^2S^e$	10.3188	10.2945	0.997645
	$(1s2s2p)^2P^o$	10.5687	10.6214	1.004986
	$(1s2s3p)^2P^o$	10.3245	10.3636	1.003787
Be <sup>+</sup>	$(1s2s2s)^2S^e$	19.8935	20.2459	1.017714
	$(1s2s3s)^2S^e$	18.5437	19.1593	1.033197
	$(1s2s2p)^2P^o$	19.7765	19.9138	1.006942
	$(1s2s3p)^2P^o$	19.2098	19.1200	0.995325
B <sup>2+</sup>	$(1s2s2s)^2S^e$	32.4376	32.6829	1.007562
	$(1s2s3s)^2S^e$	32.4517	30.6716	0.945146
	$(1s2s2p)^2P^o$	33.0987	32.2058	0.973023
	$(1s2s3p)^2P^o$	31.8765	30.6127	0.960353
C <sup>3+</sup>	$(1s2s2s)^2S^e$	48.0376	48.1209	1.001734
	$(1s2s3s)^2S^e$	44.7643	44.7249	0.999119
	$(1s2s2p)^2P^o$	45.7895	47.4970	1.037290
	$(1s2s3p)^2P^o$	44.0987	44.8103	1.016136

<sup>P</sup> Present work.

<sup>a</sup> A. K. Bhatia [14].

**Table 6.** Comparison of our results in the calculation of total energy of the  $(1s2s2p)^2P^o$  level in the lithium-like ions with other literature values. The results are expressed in Rydbergs.

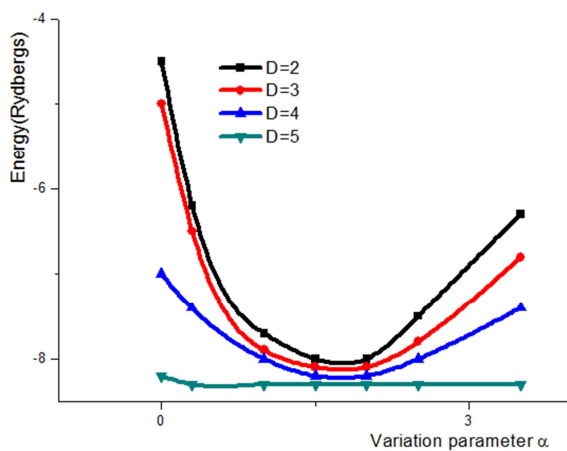
Z	Present work	Erkoç and Jansen	David and Chung	Rapport	Rapport
	$-E^P$	$-E^c$	$-E^c$	$E^c/E^P$	$E^c/E^P$
3	10.5687	10.59664	10.73696	1.002643655	1.015920595
4	19.7765	19.90236	20.13696	1.006364119	1.018226683
5	33.0987	32.21030	32.54492	0.973159066	0.983268829
6	45.7895	47.52198	47.96012	1.037835748	1.047404317
7	65.8976	65.83988	66.38402	0.999124095	1.007381452
8	86.9243	87.16696	87.81906	1.002791624	1.010293554
9	111.1765	111.50664	112.2684	1.002969512	1.009821320
10	138.3476	138.86268	139.7358	1.003723085	1.010034145

<sup>P</sup> Present work.

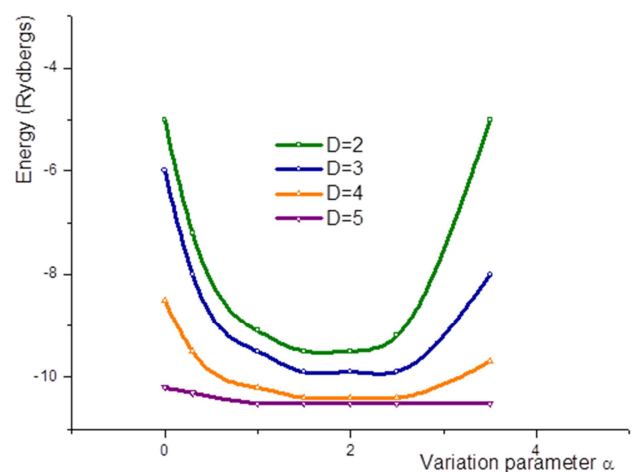
<sup>c</sup> S. Erkoç and H. J. F. Jansen. [40].

<sup>c</sup> B. F. David and K. T. Chung. [15].

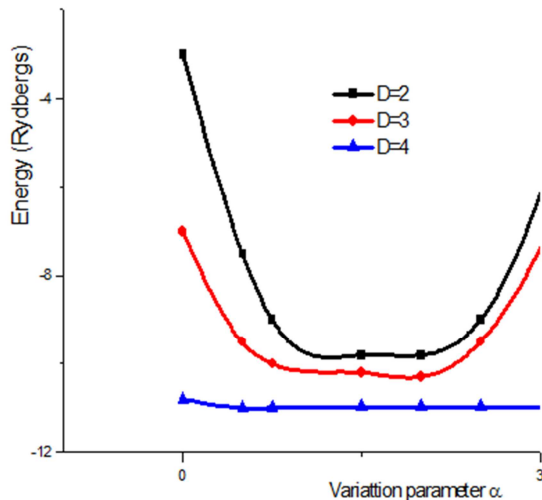
Figures 1-3 show the plots of the energy  $E=f(\alpha_i; D)$  as a function of the parameter  $\alpha_i$  and the dimension  $D$ .



**Figure 1.** Plots  $E=f(\alpha_i)$  of the energy  $E$  in terms of the variation parameter  $\alpha$  for the dimensions 2, 3, 4, 5 of the Li-like ions  $(1s4s^2)^2S^e$  state. The close similarity of the plots for  $D=4$  and  $D=5$  shows the convergence of the minima when  $D=5$ .



**Figure 2.** Plots  $E=f(\alpha_i)$  of the energy  $E$  in terms of the variation parameter  $\alpha$  for the dimensions 3, 4, 5, 6 of the Li-like ions  $(1s2s2p)^2P^o$  state. The close similarity of the plots for  $D=4$  and  $D=5$  shows the convergence of the minima when  $D=5$ .



**Figure 3.** Plots  $E=f(\alpha)$  of the energy  $E$  in terms of the variation parameter  $\alpha$  for the dimensions 2, 3, 4, 6 of the Li-like ions  $(1s2s2s)^2S^e$  state. The close similarity of the plots for  $D=4$  shows the convergence of the minima when  $D=4$ .

These plots concern the lithium atom and are performed for the  $(1s4s^2)^2S^e$ ,  $(1s2s2p)^2P^0$  and  $(1s2s2s)^2S^e$  states.

A good approximation for the eigenvalues is obtained when the minima of the functions ( $dE/d\alpha_i=0$ ) converge with increasing values of  $D$  and when the functions exhibit a plateau. As long as the functions exhibit no plateau and as long as the minima of the functions do not converge with increasing values of  $D$ , one has not yet found a good approximation.

In our calculations the exhibition of a plateau and the convergence of the minima arise when  $D=4$ . This could be seen from the figures where there is a close similarity of the plots for  $D=4$  and  $D=5$ . This similarity could be explained by the relatively weak contribution of the configurations  $(0, 0, 0)$ ;  $(0, 0, 1)$ ;  $(1, 0, 0)$  to the calculations of the eigenvalues.

It is important to notice that we have obtained a good approximation for the eigenvalues with a relatively small dimension of the basis ( $D=4$ ). Using atomic systems with three electrons and using bases as weak as possible for systems, we can observe convergence with very small dimensions. So these results are in good agreement with one aspect of electron correlation and the resemblance of the atomic levels to the rotational spectrum of Li-like ions.

## 4. Conclusion

With a relatively small dimension of the basis functions and using Hylleraas-type wave functions, we have obtained a quantitative and qualitative estimation of electron correlation effects for the ground-state and for doubly excited states of the Lithium-Like ions. It has been demonstrated the possibilities to use a new correlated wave function in the study of  $(1s^22s)^2S^e$ ,  $(1sns^2)^2S^e$ ,  $(1s2sns)^2S^e$  and  $(1s2snp)^2P^0$  doubly excited states in the Lithium-like ions.

Thus, a new correlated wave function is performed and results obtained are shown by the comparison with various available theoretical literature values. One can notice that, the merit of the

basis functions is to give the possibilities to calculate accurate energies for doubly excited states in three electron systems using separately the kinetic energy, the Coulomb potential and the Coulomb interaction between electrons. We will also note the fact that the theoretical calculation of the different terms of the disturbance Hamiltonian poses a real complex problem due to the heaviness of the mathematical formalism implemented. One of the merits of this method is to be able to get around these mathematical difficulties by a separate calculation of the different terms of the Hamiltonian which leads to very precise results. Thus our results can be used in a wide field, which goes from the physics of plasmas in intense laser field to atomic and molecular dynamics in femto second regime ( $1fs=10^{-15}s$ ) in infrared (IR). The latter field has experienced considerable development in the last decade, it is in fact linked to the technique of frequency drift amplification (Chirp Pulse Amplification) which generates very short intense pulses in the IR domain; a crucial technological advance which in 2018 won the Nobel Prize in Physics for Gérard Mourou and Donna Strickland.

## Acknowledgements

The authors would like to thank Professor Amlan Kusum Roy Division of Chemical Sciences Indian Institute of Science Education and Research (IISER) –Kolkata for providing us with several papers in this area and for his advice.

## References

- [1] Ermolaev M., J. Phys. B 17, 1069 (1984).
- [2] Fischer C. F., Comput. Phys. Commun. 64, 369 (1991).
- [3] Bronk T., Reading J. F. and Ford A. L., J. Phys. B 31, 2477 (1998).
- [4] Godunov A. L., Ivanov P. B., Shipakov V. A., Moretto-Capelle P., Bordenave-Montesquieu D. and Bordenave-Montesquieu A., J. Phys. B 33, 971 (2000).
- [5] Kuyatt C. E., Simpson J. A. and Mielczarek S. R. Phys. Rev. 138, A385 (1965).
- [6] Fano U. and Cooper J. M., Rev. Mod. Phys. 40, 441 (1968).
- [7] Skogvall B., Chesnel J.-Y., Frémont F., Lecler D., Husson X., Lepoutre A., Hennecart D., Grandin J.-P., Sulik B., Salin A. and Stolterfoht N., Phys. Rev. A 51, R4321 (1995).
- [8] Diehl S., Cubaynes D., Wuilleumier F. J., Bizau J.-M., Journel L., Kennedy E. T., Blancard C., VoKy L., Faucher P., Hibbert A., Berrah N., Morgan T. J., Bozek J., and Schlachter A. S., Phys. Rev. Lett. 79, 1241 (1997).
- [9] Diehl S., Cubaynes D., Zhou H. S., VoKy L., Wuilleumier F. J., Kennedy E. T., Bizau J.-M., Manson S. T., Blancard C., Berrah N. and Bozek J., J. Phys. B 33, L487 (2000).
- [10] Tanis J. A., Chesnel J.-Y., Frémont F., Hennecart D., Husson X., Cassimi A., Grandin J. P., Skogvall B., Sulik B., Bremer J.-H. and Stolterfoht N., Phys. Rev. Lett. 83, 1131 (1999).



- [11] Chesnel J.-Y., Tanis J. A., Sulik B., Skogvall B., Rangama J., Frémont F., Bremer J.-H., Cassimi A., Hennecart D., Hoffmann V., Husson X., Landers A. L. and Stolterfoht N., Photonic, Electronic and Atomic Collisions (XXII ICPEAC) Proceedings ed. J Burgdorfer, J Cohen, S Datz, and C Vane, pp 699-707 (2002).
- [12] R. Uptal and B. Talukdar, Phys. Scr. 59, 133 (1999).
- [13] T. J. McIlrath, T. B. Lucatorto, and R. P. Madden, Phys. Rev. Lett. 25, 1537 (1970).
- [14] A. K. Bhatia, Phys. Rev. A 18, 2523 (1978).
- [15] B. F. David and K. T. Chung, Phys. Rev. A 39, 3942 (1989).
- [16] Thakkar, A. J., Koga, T., Tanabe, T. and Teruya, H., Chem. Phys. Lett., 366, p. 95–99, (2002).
- [17] Ho Y. K., Intern. J. of Quant. Chem., 10, pp. 1077 – 1082, (1981).
- [18] Eckart, C., Phys. Rev., 36, 878, (1930).
- [19] Guillemin Jr., V. and Zener, C., Z. Phys., 61, 199, (1930).
- [20] Wilson Jr. E. B., J. Chem. Phys. 1, 210, (1933).
- [21] James, H. M., and Coolidge, A. S., Phys. Rev., 47, 700, (1935).
- [22] James, H. M., and Coolidge, A. S., Phys. Rev., 49, 688, (1936).
- [23] Weiss, A. W., Phys. Rev., 122, 1826, (1961).
- [24] Muszynska, J., Papierowska, D. and Woznicki, W., Chem. Phys. Lett., 76, 136, (1980).
- [25] King, F. W. and Shoup, V., Phys. Rev. A., 33, 2940, (1986).
- [26] King, F. W., Phys. Rev. A., 40, 1735, (1989).
- [27] King, F. W. and Bergsbaken, M. P., J. Chem. Phys., 93, 2570, (1990).
- [28] McKenzie, D. K. and Drake, G. W. F., Phys. Rev. A., 44, R6973, (1991).
- [29] Luchow, A. and Kleindienst, H., Int. J. Quantum Chem., 51, 211, (1994).
- [30] Yan, Z. C. and Drake, G. W. F., Phys. Rev. A 52, 3711, (1995).
- [31] Yan, Z. C., Tambasco, M. and Drake, G. W. F., Phys. Rev. A., 57, 1652, (1998).
- [32] Larsson, S., Phys. Rev. 169, 49 (1968).
- [33] Varshalovich, D. A., et al., Quantum Theory of Angular Momentum. Scientific Publishing Co. Ltd. (1988).
- [34] Youssou Gning, et al., Radiation Physics and Chemistry 106, 1–6 (2015).
- [35] Samarskogo, A., Edition Science, Moscow, 281 p. (1974).
- [36] J. F. Perkins, Phys. Rev. A 13, 915 (1976).
- [37] F. W. King, Phys. Rev. A 38, 6017 (1988).
- [38] F. W. King, Phys. Rev. A 40, 1735 (1989).
- [39] F. Arias de Saavedra, I. Porras, E. Buendia, F. J. Galvez, J. Phys. B 28, 3123 (1995).
- [40] S. Erkoç and H. J. F. Jansen, Phys. Rev. A 59, 2490 (1997).
- [41] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A 52, 3711 (1995).
- [42] K. T. Chung, Phys. Rev. A 44, 5421 (1991); 45, 7766 (1992). K. T. Chung and X.-W. Zhu, Phys. Scr. 48, 292 (1993).
- [43] J. Pipin and D. M. Bishop, Phys. Rev. A 45, 2736 (1992).
- [44] M. Tong, P. Jonsson, and C. F. Fischer, Phys. Scr. 48, 446 (1993).
- [45] G. Pestka and W. Woznicki, Chem. Phys. Lett. 255, 281 (1996).
- [46] I. Sakho. Chinese journal of physics vol. 48, no. 5 (2010).