

The Ground State $(1s^2s)^2S$ and the Low-lying Excited $(1s^2ns)^2S$ States Energy Calculations of Li-Like Ions Using Special Forms of the Hylleraas-Type Wave Functions

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Abstract: In this paper, we have applied the complex rotation method to the calculations energies of the ground state $(1s^2s)^2S$ and the low-lying excited $(1s^2ns)^2S$ states with $n = 3, 4$ and 5 ; of lithium and its isoelectronic series. For the ground state, the calculations were made up to $Z = 20$ and for the low-lying excited states up to $Z = 10$. These energies calculations were made using new special forms of Hylleraas-type wave functions designed by combining incomplete radial hydrogenic wave functions and Hylleraas-type wave functions. Using a numerical calculation program, the values of the resonance energies are calculated. Our results are compared with the results of ab-initio calculations using Hylleraas type wave functions and with semi-empirical results by Screening Constant by Unit Nuclear Charge (SCUNC) formalism. Analysis of the present results is achieved by calculating the ratio and the difference between our values and those of other authors. The results obtained are in good agreement with those of the theoretical methods available in the literature. This agreement shows the adequacy of our wave function with small bases to satisfactorily describe the ground state and the low-lying excited states of the three-electron atomic systems.

Keywords: Wave Function, Resonance Parameters, Correlation Factors, Resonant Width, Ground State, Low-lying Excited States, Li-like Ions

1. Introduction

Experimental and theoretical studies of the photoionization process are of fundamental importance as they have greatly increased understanding of the reactions of atoms or ions to electromagnetic radiation. Theoretical investigations on the autoionizing states of atoms and ions have developed thanks to the use of synchrotron radiation and lasers in experiments on photoabsorption and photoionization [1 - 4]. In addition, this development is also possible thanks to advanced

techniques in the measurement of photoelectron spectroscopy [5].

These autoionizing states show the importance of the electron-electron correlation, which is necessary to understand the autoionization process. In recent years, experimental and theoretical studies of the properties of multi-electron systems have been of great interest in understanding electron-electron correlation effects.

On the experimental level, transitions between the doubly excited states, which have been observed in the Li atom [6]. Beam-foil spectroscopy [7] showed a strong excitation of

these transitions. Based on these experimental observations since 1959, extensive theoretical researches on lithium isoelectric series have been the objective of physicists. Among the calculations on the ground state of lithium and its isoelectronic series, we can cite the works of Eckart [8], Guillemin and Zener [9], Wilson [10], and James and Coolidge [11, 12]. Since then, the ground state energy of Li has been refined by Weiss [13], Larsson [14], Muszynska *et al.* [15], King *et al.* [16 - 18], McKenzie and Drake [19], Luchow and Kleindienst [20], and Yan *et al.* [21, 22]. All these studies, except that of Weiss [13], use Hylleraas-type wave functions, with several terms ranging in length from 100 terms [14] to 3502 terms [22].

In addition, one of the main problems faced by physicists in studying the properties of multiple electron systems via *ab-initio* techniques is related to the complexity of the calculations, which usually require a large base set. For the $(1s^2 ns)^2S$ (with $n = 3, 4$ and 5) levels of the lithium isoelectronic sequence, Wang *et al.* [23] applied the full-core-plus correlation with multiconfiguration-interaction wave functions to compute the total energies and the first ionization potential up to $Z = 10$. These authors have also calculated, via the full-core-plus-correlation method, the energies and fine structure splitting of the $(1s^2 np)^2P$ levels (with $n = 3, 4$ and 5) of $Z = 3 - 10$ [24]. For both the $(1s^2 ns)^2S$ and $(1s^2 ns)^2P$ levels, Wang *et al.* [23, 24] included all the corrections mentioned above. Hylleraas-type (HT), wave functions containing r_{ij} factors being widely used in atomic physics to study the correlation effects between electrons and/or between electrons and the nucleus for bound and scattering states [25]. It should be noted, however, that the problems faced by physicists were the construction of an adequate wave function and the stability of a correlation factor. Those, who pushed them to make approximations to study complex atomic systems.

Thus, we are interested in this work to design new Hylleraas-type wave functions containing fewer terms named special forms of Hylleraas-type wave functions, but which provide energies with good accuracy for both ground state $(1s^2 2s)^2S$ and the low-lying excited states $(1s^2 ns)^2S$ ($n = 3, 4$ and 5) of the lithium atom and its isoelectronic series. The method of the complex rotation which is particularized from the other methods because it makes it possible to obtain at the same time the energy and width resonance will be used in this work.

In Section II, we will describe the complex Hamiltonian and the matrix elements used by the complex rotation

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

This relation (3) can be broken down into a sum of three terms as follows:

$$\hat{H} = T + C + W \quad (4)$$

method, then present the special forms of Hylleraas-type wave functions that was used for calculating energies of the ground state $(1s^2 2s)^2S$ and the low-lying excited $(1s^2 ns)^2S$ states (where $n = 3, 4$ and 5) of the lithium atom and its isoelectronic sequence. And finally, section III is devoted to the presentation of our results followed by a discussion. A comparison of our results with the available theoretical values is also made in this section.

2. Theory

2.1. Hamiltonian and Wave Function

The complex rotation method (CRM) or dilation method is widely used in atomic physics to determine the parameters of the autoionizing resonances of many electrons atomic systems governed by Coulomb interactions. It is based on the theorem of Balslev *et al.* [26]. The application of this theorem in the study of atomic resonances consists in the transformation of real Hamiltonian system $\hat{H}(r)$ to a complex Hamiltonian $\hat{H}(r, \theta)$.

The non-relativistic Hamiltonian operator for three-electron systems is given by (in *a.u.*):

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

The Hamiltonian complex $\hat{H}(r, \theta)$ obtained after changing the radial variable r into a complex variable (with θ a positive real designating the angle of rotation), comprises in addition to resonant states, a continuous spectrum formed of a series of lines in the complex plane beginning at the threshold of ionization of the residual ion of the studied atomic system, also bound discrete states which remain invariant in the rotation [27].

By this transformation, the complex Hamiltonian $\hat{H}(r, \theta)$ is written in the case of the Coulomb interaction system in the form:

$$\hat{H}(r, \theta) = \hat{T} e^{-2i\theta} + \hat{V} e^{-i\theta} \quad (2)$$

In this relation (2), \hat{T} et \hat{V} respectively denote the operators of kinetic energy and Coulomb interaction energy.

In the case of atomic systems with three electrons, the relation (2) is written in the form (*in atomic unit*):

Where:

$$\hat{T} = -\frac{1}{2} (\Delta_1 + \Delta_2 + \Delta_3) e^{-2i\theta}$$

is the kinetic energy operator of electrons;

The Laplacian is written as:

$$\Delta_i = \frac{1}{r_i^2} \frac{\partial}{\partial r_i} \left(r_i^2 \frac{\partial}{\partial r_i} \right) + \frac{1}{r_i^2 \sin \theta_i} \frac{\partial}{\partial \theta_i} \left(\sin \theta_i \frac{\partial}{\partial \theta_i} \right) + \frac{1}{r_i^2 \sin^2 \theta_i} \frac{\partial^2}{\partial \varphi_i^2} \quad (5)$$

With $i = 1, 2, 3$.

$$\hat{C} = -Z.e^{-i\theta} \left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} \right) \quad E_{res} = E_r - \frac{1}{2} \Gamma_r \quad (7)$$

is the operator of the electron-nucleus interaction energy;

Relation where, the real part E_r gives the resonance energy and the imaginary part Γ_r gives the resonance width.

$$\hat{W} = \left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) e^{-i\theta}$$

is the operator of the interaction energy between electrons.

The resonance parameters are obtained by solving the complex eigenvalue equation below:

$$\left\langle \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) \left| \hat{H}(\vec{r}, \theta) - E_{res} \right| \psi'(\vec{r}_1, \vec{r}_2, \vec{r}_3) \right\rangle = 0 \quad (6)$$

The complex eigenvalue E_{res} is in the form:

The test wave function is of the Hylleraas type. This type of wave function called the Hylleraas type special wave function has been successfully applied by Biaye et al. [28-32], Dieng et al. [33, 34], Gning et al. [35, 36] for the calculation of the excited state resonance parameters of helium and its isoelectronic series. To broaden the field of research, we have made modifications to these wave functions originally designed for two-electron atomic systems in order to adapt them to the study of three-electron atomic systems.

Thus, the Hylleraas-type special wave function that we used to calculate the ground state energy $(1s^2 2s) \ ^2S$ and the excited states $(1s^2 ns) \ ^2S$ with $n = 3, 4$ and 5 of lithium and Li-like ions of nuclear charge $Z = 3 - 10$ is defined as follows:

$$\Psi_{ijknpq}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \phi_{npq}(\vec{r}_1, \vec{r}_2, \vec{r}_3) \times \chi_{ijk}(\vec{r}_1, \vec{r}_2, \vec{r}_3) \quad (8)$$

Where $\phi_{npq}(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ are basic spatial functions and $\chi_{ijk}(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ are functions involving the spherical harmonics of the three electrons.

The basic spatial functions are conventionally of the form Hylleraas:

$$\phi_{npq}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \left\{ (3r_1 3r_2 3r_3)^{l_1} \sum_{v=0}^{n_1-l_1-1} (n_1^2 r_0^2 \alpha^2 3r_1 3r_2 3r_3)^v + (3r_1 3r_2 3r_3)^{l_3} \times \sum_{v'=0}^{n_3-l_3-1} (n_3^2 r_0^2 \gamma^2 3r_1 3r_2 3r_3)^{v'} \right\} \times r_{12}^n \cdot r_{13}^p \cdot r_{23}^q \cdot \exp(-\alpha r_1 - \beta r_2 - \gamma r_3) \quad (9)$$

The functions involving the spherical harmonics of the three electrons are of the form:

$$\chi_{ijk}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \left[r_1^i r_2^{j+L} Y_{00}^{(1)} Y_{L_{12}0}^{(2)} + (-1)^{S_{12}} r_2^i r_1^{j+L} Y_{L_{12}0}^{(1)} Y_{00}^{(2)} \right] \times r_3^k Y_{00}^{(3)} \quad (10)$$

In relations (9) and (10), r_1, r_2, r_3 are the electron-nucleus distances; r_{12}, r_{13}, r_{23} are the inter-electronic distances and r_0 the Bohr radius;

The parameters $\{i, j, k, n, p, q\}$ are non-zero positive integers. The set consisting of the six parameters $\{i, j, k, n, p, q\}$ represents a state base (i.e. configuration) of the three-electron system and obeys the condition: $i + j + k + n + p + q \leq \Omega$, where Ω is a positive integer.

The exponents α, β and γ are the nonlinear variational parameters.

n_1, n_2 and n_3 are respectively the main quantum numbers of electrons 1, 2 and 3;

l_1, l_2 and l_3 are respectively the orbital angular moments of the three electrons;

$L_{12} = l_1 + l_2$ is the angular momentum coupling the electrons 1 and 2;

S_{12} being total spin of electrons 1 and 2;

$Y_{00}^{(1)}$, $Y_{L_{12}0}^{(2)}$, and $Y_{00}^{(3)}$ are respectively the spherical harmonics of electron 1, 2 and 3.

The correlation factor r_{ij}^n ($i, j = 1, 2, 3$ with $i < j$) model

$$r_{ij}^n = 4\pi \sum_{l=0}^{\infty} \frac{1}{2l+1} \frac{\binom{-n}{2}_l}{\binom{1}{2}_l} \times \frac{r_i^l}{r_j^{l-n+2}} \times \left[r_j^2 - \frac{(2l-n)(1+n)}{2(2l+3)} \times r_i^2 \right] \times (Y_l(\Omega_i) Y_l(\Omega_j)) \quad (11)$$

$$Y_l(\Omega_i) Y_l(\Omega_j) = \sum_{m=-l}^l Y_{l,m}^*(\Omega_i) Y_{l,m}(\Omega_j) \text{ with } \Omega_i = (\theta_i, \varphi_i)$$

2.2. Calculation Procedures

The test wave functions used for the different states are all Hylleraas-type. Unfortunately, for the states studied in this work, an appropriate fixed set of exponential parameters is not available. The restriction $\alpha = \beta$ has been adopted and the parameters $\{\alpha = \beta$ and $\gamma\}$ for each state are determined by optimizing the energy for the small-base wave function. An algorithm that used analytic expressions of the matrix elements for all states studied ($1s^2 2s$)²S and ($1s^2 ns$)²S is designed. This calculation program is written in Maxima. At the start of the calculation procedure, we initialize the angle of rotation θ and the parameters ($i, j, k, n,$

p, q) satisfying the conditions ($i, j, k, n, p, q > 0$ and $i + j + k + n + p + q = \Omega$) and then we vary the positive exponential parameters.

Thus, we first fixed the base Ω to 9, the rotation angle at $\theta = 0.30$ and we minimize the energy with respect to the exponential parameters. A second test is done keeping the same exponential parameters but this time increasing the base Ω to 12 and minimizing the energy relative to the rotation angle θ . The ground state ($1s^2 2s$)²S energy of lithium $E(\Omega)$ obtained in the two tests are listed in the following Table 1:

Table 1. Convergence of non-relativistic energies for the ground state ($1s^2 2s$)²S of lithium, in atomic units.

Ω	$E(\Omega)$	θ	$\alpha = \beta$	γ
9	7.478037459100333	0.300		
12	7.477696606665282	0.683	6.850	0.282

The energy obtained with the base $\Omega = 9$ is 6.5×10^{-6} greater than -7.478031 a.u. from the 92-term Hylleraas-type wave function of Ho [25] and lower by 3.55×10^{-5} than -7.4780730 a.u. from Bunge [38], whereas that obtained with the base $\Omega = 12$ is lower by 3.34×10^{-4} than the 92-term Hylleraas-type wave function of Ho [25] and lower by 3.76×10^{-4} than the value from Bunge [38]. Consequently, in our calculations of energies for the ground state and low-lying excited states ($1s^2 ns$)²S with $n = 3, 4$ and 5 of lithium

and its isoelectronic series, we set the size of the wave functions Ω to 9.

The rotation angle θ is changed according to Z by increments of $+0.1$ up to $Z = 15$, then by increments of $+0.05$ from $Z = 16$ to 20 for the ground state ($1s^2 2s$)²S and by increments of $+0.05$ for the low-lying excited states ($1s^2 ns$)²S states for all Z . The final set of the positive exponentials parameters α, β and γ used for all the series studied is collected in Table 2.

Table 2. Exponents parameters employed for the ground state ($1s^2 2s$)²S and excited states ($1s^2 ns$)²S (with $n = 3, 4$ and 5) wave functions for members of the Lithium and its isoelectronic series.

Z	Etats							
	$(1s^2 2s)^2S$		$(1s^2 3s)^2S$		$(1s^2 4s)^2S$		$(1s^2 5s)^2S$	
	$\alpha = \beta$	γ						
3	6.850	0.282	10.475	0.145	11.938	0.197	11.150	0.263
4	8.558	0.266	12.491	0.157	15.020	0.208	14.868	0.266
5	9.981	0.307	14.430	0.169	17.560	0.210	18.055	0.270
6	11.125	0.300	16.240	0.179	19.945	0.226	20.973	0.280
7	12.380	0.329	17.983	0.190	22.250	0.241	23.750	0.302
8	13.633	0.350	19.800	0.211	24.516	0.250	26.467	0.312
10	14.930	0.365	21.395	0.217	26.790	0.265	28.526	0.320

3. Results and Discussions

The results obtained in the present calculations energies for the ground state ($1s^2s$) 2S up to $Z = 20$ and low-lying excited states ($1s^2ns$) 2S (with $n = 3, 4$ and 5) up to $Z = 10$ of lithium and its isoelectronic series are listed in Table 3.

Table 3. Present energy ($-E^P$) of the ground state ($1s^2s$) 2S and low-lying excited states ($1s^2ns$) 2S with $n = 3, 4$ and 5 of Li-like ions. The results are expressed in a.u. ($1 \text{ a.u.} = 2 \text{ Ryd} = 27.211396 \text{ eV}$).

Z	$-E^P$			
	($1s^2s$) 2S	($1s^23s$) 2S	($1s^24s$) 2S	($1s^25s$) 2S
3	7.478037459	7.353119890	7.318532483	7.303710557
4	14.324269223	13.919308139	13.798725495	13.744477468
5	23.425215050	22.603664413	22.342163122	22.225782127
6	34.776775070	33.401418021	32.947198786	32.747035807
7	48.379836350	46.300561263	45.615081485	45.308244838
8	64.225096275	61.299037000	60.346472351	59.909417865
9	82.332917421	78.445180730	77.140741111	76.550996236
10	102.672139407	97.680943378	95.995086360	95.231523454
11	125.294516838			
12	150.137102687			
13	177.240152605			
14	206.567456533			
15	238.189137911			
16	272.059318280			
17	308.150321379			
18	346.493612924			
19	387.089626633			
20	429.953087132			

Table 4. Comparison of the present total energies ($-E^P$) of the ground state ($1s^2s$) 2S of lithium and its isoelectronic series ($Z = 3 - 20$) with other results. The results are expressed in a.u. ($1 \text{ a.u.} = 2 \text{ Ryd} = 27.211396 \text{ eV}$).

Z	Present work	Sakho and al. [40]	Yan and al. [22]	Thakkar and al. [39]	Chung and al. [42]	Ho [25]	E^V/E^P	E^S/E^P	E^C/E^P
3	7.478037459	7.477749400	7.478060323	7.478059609	7.478059700	7.4780310	1.0000	1.0000	1.0000
4	14.324269223	14.32524798	14.32476318	14.32475926	14.32476100	14.3246960	1.0000	1.0001	1.0000
5	23.425215050	23.42774331	23.42460572	23.42460310	23.42460310	23.4245230	1.0000	1.0001	1.0000
6	34.776775070	34.78122732	34.77551128	34.77550835	34.77550820	34.7754180	1.0000	1.0001	1.0000
7	48.379836350	48.38475520	48.37689832	48.37689500	48.37689490	48.3767980	0.9999	1.0001	0.9999
8	64.225096275	64.23809034	64.22854208	64.22853918	64.22853850	64.2284350	1.0001	1.0002	1.0001
9	82.332917421	82.34119050	82.33033810	82.33033508	82.33033480		1.0000	1.0001	1.0000
10	102.672139407	102.6940698	102.6822315	102.6822283	102.6822278		1.0001	1.0002	1.0001
11	125.294516838	125.2967557	125.2841908	125.2841875			0.9999	1.0000	
12	150.137102687	150.1492770	150.1361966	150.1361932			1.0000	1.0001	
13	177.240152605	177.2516594	177.2382366	177.2382331			1.0000	1.0001	
14	206.567456533	206.6069240	206.5903022	206.5902987			1.0001	1.0002	
15	238.189137911	238.2060891	238.1923876				1.0000	1.0001	
16	272.059318280	272.0581691	272.0444888				0.9999	1.0000	
17	308.150321379	308.161760	308.1466024				1.0000	1.0000	
18	346.493612924	346.5121209	346.4987262				1.0000	1.0001	
19	387.089626633	387.1140110	387.1008583				1.0000	1.0001	
20	429.953087132	429.9658537	429.9529975				1.0000	1.0000	

In Table 5, we compared our present results ($-E^P$) of the low-lying excited states ($1s^2ns$) 2S (with $n = 3, 4$ and 5) of the lithium and its isoelectronic series ($Z = 3 - 10$) with the theoretical results of Sakho [44] who applied the Screening Constant by Unit Nuclear Charge method (SCUNC-method), King [45] who applied the variational method on Hylleraas-type wave functions and Wang and al. [23, 24] who applied the Full-Core-Plus-Correlation (FCPC) with

Table 4 shows a comparison of our present results ($-E^P$) of the ground state ($1s^2s$) 2S of lithium and its isoelectronic series with the theoretical results of Yan and al. [22] which used the variational method of 3502-term Hylleraas-type wave function ($Z = 3 - 15$) and expansion method Z^{-1} ($Z = 16 - 20$), Thakkar and al. [39] also used 50-term Hylleraas-type wave functions. Ho [25] who used Hylleraas-type wave functions at one spin of 60-term and 92-term, Sakho and al. [40] who used the Screening Constant by Unit Nuclear Charge method (SCUNC) method and Chung and al. [41 - 43] used the method of Full-Core-Plus-Correlation (FCPC). This comparison with various theoretical data which we have just quoted indicates a good agreement between the calculations. Indeed, the ratio (E^V/E^P , E^S/E^P and E^C/E^P) between the results of these authors and our results is higher than 0.9999 and lower than 1.0002 for all the ions studied. Here again, we can perceive that our results are closer to the other data up to $Z = 10$ where the maximum energy difference between the present results and the theoretical data are less than 0.0040 a.u., nevertheless, for $Z \geq 10$ the energy differences never exceeded 0.0400 a.u. because the maximum energy differences with the values of Yan and al. [22], and Sakho and al. [40] are respectively 0.0228 and 0.0395. It should be mentioned that our data correspond more to *ab-initio* calculations using for the most part Hylleraas-type wave functions [22, 25, 39] than *semi-empirical* results of Sakho [40].

multiconfiguration-interaction wave functions. Here again, the agreement between the calculations is very good because the maximum energy differences in the ($1s^23s$) 2S , ($1s^24s$) 2S and ($1s^25s$) 2S states are respectively less than 0.0095 a.u., 0.0008 a.u and 0.0003 a.u. In addition, the ratio between the results of the above authors and our results is more than 0.9997 and less than 1.0003. As in the case of the ground state, our data for low-lying excited states ($1s^2ns$) 2S (with n

= 3, 4 and 5) agree more with *ab-initio* calculations using empirical results of Sakho [44]. Hylleraas-type wave functions [23, 24, 25] than the *semi-*

Table 5. Comparison of the present total energies ($-E^P$) of the low-lying excited states ($1s^2 ns$) 2S when $n = 3, 4$ and 5 of lithium and its isoelectronic series ($Z = 3 - 10$) with other results. The results are expressed in a.u. ($1 \text{ a.u.} = 2 \text{ Ryd} = 27.211396 \text{ eV}$).

Z	Etats	E^P	E^W	E^S	E^K	$ \Delta E ^W$	$ \Delta E ^S$	$ \Delta E ^K$
3	$1s^2 3s$	7.353120	7.354098	7.354090	7.354076	0.0010	0.0010	0.0010
	$1s^2 4s$	7.318532	7.318530	7.318520	7.318315	0.0000	0.0000	0.0002
	$1s^2 5s$	7.303711	7.303551	7.303650	7.301943	0.0002	0.0001	0.0018
4	$1s^2 3s$	13.919308	13.922789	13.918900	13.922764	0.0035	0.0004	0.0035
	$1s^2 4s$	13.798725	13.798714	13.797000	13.798662	0.0000	0.0017	0.0001
	$1s^2 5s$	13.744477	13.744631	13.743910	13.744577	0.0002	0.0006	0.0001
5	$1s^2 3s$	22.603664	22.603751	22.597990	22.603724	0.0001	0.0057	0.0001
	$1s^2 4s$	22.342163	22.341831	22.340120	22.341779	0.0003	0.0020	0.0004
	$1s^2 5s$	22.225782	22.225835	22.225940		0.0001	0.0002	
6	$1s^2 3s$	33.401418	33.396215	33.389770	33.396188	0.0052	0.0116	0.0052
	$1s^2 4s$	32.947199	32.947571	32.946800	32.947524	0.0004	0.0004	0.0003
	$1s^2 5s$	32.747036	32.747047	32.748830		0.0000	0.0018	
7	$1s^2 3s$	46.300561	46.299964	46.293540	46.299936	0.0006	0.0070	0.0006
	$1s^2 4s$	45.615081	45.615857	45.616580	45.615809	0.0008	0.0015	0.0007
	$1s^2 5s$	45.308245	45.308253	45.312230		0.0000	0.0040	
8	$1s^2 3s$	61.299037	61.314913	61.308990	61.314886	0.0159	0.0100	0.0158
	$1s^2 4s$	60.346472	60.346664	60.349240	60.346614	0.0002	0.0028	0.0001
	$1s^2 5s$	59.909418	59.909458	59.915930		0.0000	0.0065	
9	$1s^2 3s$	78.445181	78.441025	78.435910	78.440999	0.0042	0.0093	0.0042
	$1s^2 4s$	77.140741	77.139982	77.144650	77.139930	0.0008	0.0039	0.0008
	$1s^2 5s$	76.550996	76.550648	76.559840		0.0003	0.0088	
10	$1s^2 3s$	97.680943	97.678282	97.674200	97.678256	0.0027	0.0067	0.0027
	$1s^2 4s$	95.995086	95.995804	96.002730	95.995752	0.0007	0.0076	0.0007
	$1s^2 5s$	95.231523	95.231829	95.243890		0.0003	0.0124	

E^P : Present travail, E^W : Wang and al.[23] E^S : Sakho [44] E^K : King [45].

It should be mentioned that for all the states studied, the exponential parameter α (or β) for the $1s^2$ -shell core electrons (internal electrons) varies widely depending on the state for the same Z but also for different values of Z . The exponential parameter γ describing the valence electron varies slightly, depending on the excited state for the same Z .

4. Conclusion

With a relatively small basic dimension of the functions and using Hylleraas-type wave functions, we have obtained the ground state ($1s^2 2s$) 2S and the low-lying excited ($1s^2 ns$) 2S states of energies of Li-Like. The present work provides the first calculations on the ground state and low-lying excited states energies of Lithium and its isoelectronic series using Hylleraas-type wave functions in our laboratory. Generally, our calculations for the total energies of the ($1s^2 2s$) 2S and ($1s^2 ns$) 2S (with $n = 3, 4$ and 5) of Li-Like are in good agreement with existing theoretical results. This chord shows the adequacy of our Special Forms of the Hylleraas-Type Wave Functions with small basis to satisfactorily describe the ground state and low-lying excited states of the three-electron atomic systems. The few differences noted can be explained by the fact that we have used, in this work, the largest sets of exponential parameters obtained by minimizing energy. However, several approaches to improve the speed of convergence are, therefore, interesting to try. Although this would require much time and powerful computers since the integrals involved would be quite heavy,

we have planned to do other works on Lithium energy with improved wave functions.

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