Société Ouest Africaine de Physique -SOAPHYS.
West African Physical Society- WAPS.

ISSN 2630-0958

Journal de Physique de la Soaphys

J. P. Soaphys

Volume 2, Numéro 2 - Décembre 2020

Journal de Physique de la Soaphys

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SOMMAIRE

Thermal destruction of gas generated from household waste …… C20A15 :1-5
Palm et al.,

Energy calculations of the $(2p^2\ 1D)$; $(3d^2\ 1G)$ and $(4f^2\ 1I)$ doubly excited states of helium isoelectronic sequence ($Z \leq 20$) via the modified atomic orbital theory …… C20A16 :1-7
Sow

Potentiel érosif de la pluie : identification du meilleur estimateur d'énergie cinétique de la pluie à partir des données de dropsize distribution (DSD) de pluies mesurées au nord-ouest du bénin …… C20A17 :1-5
Adjikpe et al.,

Le carbone 14 (^{14}C) un traceur idéal pour la surveillance dela pollution atmosphérique en dioxyde de carbone (CO_2) anthropogénique dans la zone de Dakar …… C20A18 :1-8
Sène et al.;

Influences of local materials on the building behavior and evaluation of the cooling loads …… C20A19 :1-7
Amadou et al.,

Evaluation du potentiel en petite hydroelectricite du bassin versant de wassadou en utilisant le modele hydrologique SWAT …… C20A20 :1-9
Ndiaye et al.,

Modélisation de la distribution granulométrique des gouttes de pluie par la loi gamma généralisée …… C20A21 :1-5
Kougbeagbede et al.,

Adaptive proportional integral controller based on ann for DC link voltage control single-phase inverter connected to grid …… C20A22 :1-6
Traoré et al.,

Evaluation du pouvoir methanogene de la jacinthe d'eau sur le lac Nokoué a ganvie au Bénin …… C20A23 :1-5
Dohou et al.,

Evaluation du potentiel de production du biogaz emanant des déchets organiques : cas de Bamako …… C20A24 :1-6
Koné et al.,

Modélisation du rayonnement solaire global incident sur un plan horizontal et incliné par quatre modèles semi-empiriques sur le site de la ville de Ouagadougou …… C20A25 :1-9
Ouédraogo et al.,

Modélisation et simulation d'un bâtiment classique vers un bâtiment à energie positive (BEPOS) …… C20A26 :1-7
Sawadogo et al.,

Recherche de tendances récentes dans les séquences sèches : cas des stations synoptiques du Bénin …… C20A27 :1-17
Gnihatin et al.,

Theoretical and experimental analysis of a boost converter …… C20A28 :1-9
Badiane et al.,

J. P. Soaphys, Vol 2, N°2 (2020) C20A16
http://dx.doi.org/10.46411/jpsoaphys.2020.02.16

Journal de physique de la SOAPHYS
http://www.soaphys.org/journal/
ISSN Print : 2630-0958

ENERGY CALCULATIONS OF THE (2P^2 ^{1}D); (3D^2 ^{1}G) AND (4F^2 ^{1}I) DOUBLY EXCITED STATES OF HELIUM ISOELECTRONIC SEQUENCE ($Z \leq 20$) VIA THE MODIFIED ATOMIC ORBITAL THEORY

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INFOS SUR L'ARTICLE

Historique de l'article:
Reçu le : 26 novembre 2020
Réçu en format revisé le : 15 mars 2021
Accepté le : 20 mars 2021

Keywords : Modified Atomic Orbital Theory, Variational Calculations, Correlated Wavefunction, Energies, , Doubly Excited States, Helium Isoelectronic Sequence, Atomes and Ions.

ABSTRACT

We report in this paper the total energies of the 2p^2 ^{1}D, 3d^2 ^{1}G, 4f^2 ^{1}I doubly excited states of Helium isoelectronic sequence with nuclear charge $Z \leq 20$. Calculations are performed using the Modified Atomic Orbital Theory (MAOT) [1;2] in the framework of a variational procedure. The purpose of this study required a mathematical development of the Hamiltonian applied to Slater-type wave function [3] combining with Hylleraas-type wave function [4]. The study leads to analytical expressions which are carried out under special MAXIMA computational program. This proposed MAOT variational procedure, leads to accurate results in good agreement as well as with available other theoretical results than experimental data. In the present work, a new correlated wave function is presented to express analytically the total energies for each 2p^2 ^{1}D, 3d^2 ^{1}G, 4f ^{2} ^{1}I Doubly Excited States (DES) in the He-like systems. The present accurate data may be a useful guideline for future experimental and theoretical studies in the (nl^2) systems.

I. INTRODUCTION

For the doubly excited states in He-like ions, since the early experiment [5] and theoretical explanation [6], Doubly Excited States (DES) of Helium isoelectronic sequence have been the target of a number of theoretical approaches. Greatest attention have been concentrated on studying symmetric DES (nl^2) with excited electrons having equal values of principal quantum number n (intrashell states) where the electronic correlation effect may be predominant [7]. The investigations of the intrashell states of two-electrons systems are advanced and due to the group theoretical method [8] which allowed intrashell states to be approximatively classified and some of these properties studied [9]. Theoretical investigations of (nl^2) doubly excited states are performed by using various method. The projection operator method and group theoretical methods have been used for energies calculations of the 2s^2, 2p^2 states in Helium-like ions. Time independent variational perturbation [10] was applied for total energies calculations of the 2s^2, 2p^2 and 3d^2 states in He, Li+, Be^{2+} and B^{3+}. The correlation part of the energies for the 2s^2, 2p^2, 3s^2, 3p^2 , 3d^2 states in He isoelectronic series have been investigated by using perturbation theory [11]. The Screening Constant by Unit Nuclear charge (SCUNC) method [12] used a semi-empirical procedure to calculate (ns^2) ^{1}S^e , (np^2) ^{1}D^e and (Nsnp) ^{1}P° excited state of He-like ions. Recently the Modified Atomic Orbital Theory (MAOT) has been applied successfully in the studies of high lying ^{1,3}P° of He-like ions [13]. In this paper, we apply the MAOT variational procedure, to calculate the total energies of the singlet DES 2p^2 ^{1}D, 3d^2 ^{1}G and 4f^2 ^{1}I Doubly Excited States of He isoelectronic sequence. Our present procedure leads to analytical expression which are carried out under MAXIMA computational program. Our energies positions are compared to other available theoretical and experimental data.

II. THEORY

2.1. Brief Description of the MAOT Formalism

In the framework of Modified Atomic Orbital Theory (MAOT), total energy E of ($\nu\ell$)-given orbital is expressed in the form [13]:

$$E(\upsilon\ell) = -\frac{\left[Z-\sigma(\ell)\right]^2}{\upsilon^2} \qquad (1)$$

In this equation (1), Z is a nuclear charge of the considered element, υ is a principal quantum number and $\sigma(\ell)$ is a screening constant of ℓ given orbital.

For an atomic system of several electrons M, the total energy E is given by (in Rydberg):

$$E = -\sum_{i=1}^{M} \frac{\left[Z - \sigma_i(\ell)\right]^2}{\upsilon_i^2} \qquad (2)$$

In this equation (2), $\sigma_i(\ell)$ and υ_i are respectively a screening constant and a principal quantum number of an electron i.

With respect to the usual spectroscopic notation $(N\ell, N\ell')\,{}^{2S+1}L^{\pi}$, this equation becomes

$$E = -\sum_{i=1}^{M} \frac{\left[Z - \sigma_i\left({}^{2S+1}L^{\pi}\right)\right]^2}{\upsilon_i^2} \qquad (3)$$

In the photoionization study, energy resonances are generally measured relatively to the E∞ converging limit of a given $({}^{2S+1}L_J)nl$-Rydberg series. For these states, the general expression of the energy resonances is given by the formula [14] presented previously (in Rydberg units):

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1\left({}^{2S+1}L_J\right) - \sigma_2\left({}^{2S+1}L_J\right) \times \frac{1}{n} - \sigma_2^{\alpha}\left({}^{2S+1}L_J\right) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2 \qquad (4)$$

In this equation *m* and *q* *(m < q)* denote the principal quantum numbers of the $({}^{2S+1}L_J)nl$-Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i({}^{2S+1}L_J)$-screening constants, s represents the spin of the *nl*-electron (s = ½), *E∞* is the energy value of the series limit generally determined from the NIST atomic database, E_n denotes the corresponding energy resonance, and Z represents the nuclear charge of the considered element. The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k \frac{1}{f_k(n,m,q,s)}$ term. The correct expression of this term is determined iteratively by imposing general Eq. (4) to give accurate data with a constant quantum defect values along all the considered series. The value of *α* in the σ_2 of the last term is fixed to 1 and 2 during the iteration. The quantum defect *δ* is calculated from the standard formula

$$E_n = E_\infty - \frac{RZ_{core}^2}{(n-\delta)^2} \qquad (5)$$

In this equation (5), *R* is the Rydberg constant, Z_{core} represents the electric charge of the core ion.

Z_{core} is directly obtained by the photoionization process from an atomic X system $X + h\nu \rightarrow X^{p+} + pe^-$

$f_k = f_k\left({}^{2S+1}L_J, n, s, m, q\right)$ are screening constants to be evaluated empirically with k taking the values from 1 to q.

L_J: denote the considered quantum state *(S, P, D, F…..).*

2.2. Variational procedure of calculations

We constructed the basis wave functions below by combining Slater-type wave function [3] and Hylleraas-type wave functions [4]:

$$\phi_{jkmn}\left(\vec{r}_1, \vec{r}_2\right) = (r_1 r_2)^{(\upsilon-1)} \times \exp\left(-\xi(r_1+r_2)\right)(r_1+r_2)^J (r_1-r_2)^K \left|\vec{r}_1 - \vec{r}_2\right|^M$$

(6)

Where $\xi = \frac{Z-\sigma}{\upsilon \times a_0}$ is a variational parameter

Z, σ, υ and a_0 are respectively the nucleus charge number, the screening constant, the principal quantum number and Bohr's radius

With $\left|\vec{r}_1 - \vec{r}_2\right| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12}}$

Where $\vec{r}_1$ and $\vec{r}_2$ denote the positions of the two electrons;

r_1 and r_2 are respectively used for $\left|\vec{r}_1\right|$ and $\left|\vec{r}_2\right|$, J, K, M are Hylleraas parameters with $(J, K, M \geq 0)$.

J takes into account the distance of the two electrons from the nucleus, *K* takes into account the approximation of the two electrons from the nucleus; *M* takes into account the distance between the two electrons.

The final form of the wave function of the singlet doubly excited state can be written as follow:

$$\Psi_n\left(\vec{r}_1, \vec{r}_2\right) = \sum_{jkm} \beta_{jkm} \phi_{jkmn}\left(\vec{r}_1, \vec{r}_2\right) \qquad (7)$$

Where the coefficients β_{jkm} are determined by solving the Schrödinger equation:

$$H\Psi_n\left(\vec{r}_1, \vec{r}_2\right) = E\Psi_n\left(\vec{r}_1, \vec{r}_2\right)$$

(8)

Where the Hamiltonian operator H has the form:

$$H = T + C + W \qquad (9)$$

with

$$T = \frac{-\hbar^2}{2m}\left(\nabla_1 + \nabla_2\right);\ C = -\left(\frac{Ze^2}{r_1} + \frac{Ze^2}{r_2}\right);\ W = \frac{e^2}{\left|\vec{r}_1 - \vec{r}_2\right|} \qquad (10)$$

Where T is the kinetic energy, C is the Coulomb potential between the atomic nucleus and the two electrons, W is the Coulomb interaction between electrons.

In the Hamilton operator we neglected all magnetic and relativistic effects together with the motion of the atomic nucleus.

In this equation (10), Z is the nuclear charge ∇_1 is the Laplacian with reference to the coordinates of the vector radius $\mathbf{r_1}$ which detect the position of the electron 1. ∇_2 Laplacian defines the coordinates of the vector radius $\mathbf{r_2}$ which detect the position of the electron 2 and $\left|\vec{r_1}-\vec{r_2}\right|$ inter- electronic distance.

The representation of the Schrödinger equation on the non-orthogonal basis leads to the general eigenvalue equation [15];

$$\sum_{(j,k,m),(j'k'm')}\left(H_{JKMnl}-EN_{JKMnl}\right)=0 \tag{11}$$

With $J=j+j'$; $K=k+k'$; $M=m+m'$

$N_{JKMnl}=\left\langle \phi_{jkmnl}\middle|\phi_{j'k'm'nl}\right\rangle$: is the normalization factor

$H_{JKMnl}=\left\langle \phi_{jkmnl}\middle|H\middle|\phi_{j'k'm'nl}\right\rangle$: is the matrix elements of Hamilton operator

$$H_{JKMnl}=T_{jkm,j'k'm'nl}+C_{JKMnl}+W_{JKMnl} \tag{12}$$

$T_{jkm,j'k'm'nl}$: is the matrix elements of the kinetic Energy operator of the two electrons

C_{JKMnl} : is the matrix elements of the Coulombian interaction Energy operator between the nucleus and the two electrons.

W_{JKMnl} : is the matrix elements of the Coulombian interaction Energy operator between the two electrons

E : is the eigenvalue of the energy given as below:

$$\left\langle E\right\rangle=\frac{\left\langle H_{JKMnl}\right\rangle}{\left\langle N_{JKMnl}\right\rangle}=\frac{\left\langle T_{JKMnl}\right\rangle+\left\langle C_{JKMnl}\right\rangle+\left\langle W_{JKMnl}\right\rangle}{\left\langle N_{JKMnl}\right\rangle} \tag{13}$$

By following the form of the basis wave function above (6), we have constructed for each state a special wave function and then calculated the matrix elements N_{JKMnl} $,C_{JKMnl}$, W_{JKMnl}, $T_{jkm,j'k'm'nl}$

The mathematical development of the Hamiltonian applied to each wave function of each state leads to simplified analytical expressions of each matrix elements which are carried out under MAXIMA computational program.

MAXIMA is a computer algebra system for the manipulation of symbolic and numerical expressions, including differentiation, integration, ordinary differential equations, and matrix elements. MAXIMA yields high precision numeric results by using exact fractions, arbitrary precision integers, and variable precision floating point numbers. Our MAXIMA source code is compiled on windows systems.

At the beginning, the variational parameter ξ is determined. Thus for each value of Z and n, we know a limited area of the variational parameter ξ and the program will calculate directly the eigenvalue E. To obtain the minimum eigenvalue in which we are interested and quoted in tables 1-3, the variational parameter ξ and the Hylleraas parameters (J, K, M) are slightly varied that exhibit a plateau for the energy $E=f(\xi,J,K,M)$.

III. RESULTS AND DISCUSSIONS

The main results of our calculations for the variational parameter ξ and energies of the $2p^2\ {}^1D$, $3d^2\ {}^1G$ and $4f^2\ {}^1I$ Doubly Excited State of helium isoelectronic sequence ($Z \leq 20$) are quoted in Tables 1-3. Our present results are compared with other theoretical calculations and experimental data. The experimental measurements [18; 19] are published in Rydberg. Then our results are also converted into Rydberg for direct comparison by using the infinite Rydberg 1Ry = 0.5 a.u = 13.605698 eV.

In table 1, we reported the value of the variational parameter ξ and total energies for $2p^2\ {}^1D$ doubly excited states of He-like ions up to $Z = 20$. For this state, comparison shows that MAOT results agree well with the theoretical results of the variational method of Biaye et al. [4]; the time-dependent variation-perturbation theory (TDVPT) of Ray et al. [10], the variational method of Ivanov et al. [11], the screening constant by Unit nuclear charge method of Sakho et al. [12], density-functional calculation of Roy et al. [16], the Complex-coordinate calculation [17] and also the experimental data of [18] [19]. For $Z \leq 10$, it can be seen that the MAOT results agree very well with the listed literature data. The very good agreement between the calculations should be mentioned. Comparison indicates that results agree well with each other. In addition, we calculated the energy of the ion Hydrogen H^- where there is no available data for comparison. For Z=10, our results at -46.5156 Ry are compared with those of Biaye et al. [4], of Ivanov et al. [11], and Sakho et al. [12] respectively at -46.49816 Ry; -46.53271 Ry and -46.46435 Ry. These results show that our MAOT calculations match more with those from the SCUNC formalism of Sakho and the variational method. Thus, this good agreement allowed us to expect our results up to $Z = 20$ to be also accurate. We mentioned that our MAOT calculations, which include more correlation than all the other calculations [4, 12, 16], should in principal provide the most precise lifetimes theoretically.

Table 1: *Variational parameter ξ and total energies E for the $2p^2\,{}^1D$ doubly excited states. The values are reported in Rydberg (Ry). 1Ry= 13.605698 eV.*

		Theory						Experiment	
Z	ξ	$-E^{MAOT}$	$-E^{SCUNC}$	$-E^{BIA}$	$-E^{c}$	$-E^{g}$	$-E^{h}$	$-E^{e,f}$	$-E^{Ray}$
1	0.3244	0.2335							
2	0.8244	1.3841	1.4052	1.4097			1.4266	1.4052^{e}	1.3728
3	1.3244	3.5398	3.5418	3.5565	3.5110	3.5411	3.5565	3.5396^{f}	3.3906
4	1.8244	6.6838	6.6788	6.6993	6.6545	6.6751	6.6861		6.5097
5	2.3244	10.8132	10.8153	10.8403	10.7976	10.8072	10.8160		10.6266
6	2.8244	15.9892	15.9514	15.9793			15.9455		
7	3.3244	22.0819	22.0885	22.1186			22.0753		
8	3.8244	29.1999	29.2252	29.2568			29.2046		
9	4.3244	37.3396	37.3615	37.3946			37.3350		
10	4.8244	46.5156	46.4981	46.5327			46.4643		
11	5.3244	56.6209							
12	5.8244	67.7463							
13	6.3244	79.9033							
14	6.8244	93.0931							
15	7.3244	107.2076							
16	7.8244	122.3587							
17	8.3244	138.4988							
18	8.8244	155.6603							
19	9.3244	173.8364							
20	9.8244	193.0401							

E^{MAOT}: Energy E of the Modified Atomic Orbital Theory (MAOT), present work; E^{SCUNC} [12] ; E^{BIA} [4]; E^{Ray} Experimental data [10]; E^{c} [16]; E^{g} [17]; E^{h} [11]; E^{e} Experimental data [18] ; E^{f} Experimental data [19] :.

Table 2 indicates the present MAOT calculation for the $3d^2\,{}^1G$ DES that are compared with those of the variational method of Biaye et al. [4]; the Time-Dependent Variation-Perturbation Theory (TDVPT) of Ray et al. [10], the variational method of Ivanov et al. [11], the Screening Constant by Unit Nuclear Cherge (SCUNC) of Sakho [20] and the pseudo- potential-Feshbach method of Bachau et al. [21].

Table 2: *Variational parameter ξ and total energies E for the $(3d^2\,{}^1G)$ doubly excited states. The values are reported in Rydberg (Ry). 1Ry= 13.605698 eV.*

	Theory							
Z	ξ	$-E^{MAOT}$	$-E^{Sakho}$	$-E^{a}$	$-E^{b}$	$-E^{c}$	$-E^{d}$	$-E^{Ray}$
1	0.2162	0.0152	-	-	-	-	-	-
2	0.5495	0.6260	0.6104	0.6166	0.6308	0.6303	0.5849	0.6232
3	0.8829	1.6004	1.5486	1.5538	1.5837	1.5618	1.5247	1.4601
4	1.2162	2.9529	2.9313	2.9320	2.9762	2.9377	2.9085	2.8421
5	1.5495	4.7596	4.7585	4.7540	4.8105	4.7581	4.7360	4.6669
6	1.8829	7.1927	7.0301	7.0180	7.0875	7.0229		
7	2.2162	9.8973	9.7461	9.7280	9.8079	9.7321		
8	2.5495	13.0334	12.9066	12.882	12.9718	12.8858		
9	2.8829	16.5999	16.5116	16.4800	16.5797	16.4840		
10	3.2162	20.5969	20.5609	20.5200	20.6316	20.5265		
11	3.5495	25.0246						
12	3.8829	29.8814						
13	4.2162	35.1721						
14	4.54959	40.8918						
15	4.88293	47.0424						
16	5.21626	53.6234						
17	5.54959	60.6351						
18	5.88293	68.0777						
19	6.21626	75.9507						
20	6.54959	84.2544						

E^{MAOT}: Energy E of the Modified Atomic Orbital Theory (MAOT), present work; E^{sakho} [20] ; E^{a} [21] ; E^{b} [4]; E^{c} [11]; E^{d} (Ho, 1989) as quoted in [4]; E^{Ray} [10] ;

Here, except the ion Hydrogen H^-(Z =1) where there is no available results, the agreements between the calculation are generally good up to $Z = 5$. Thus for $5 < Z \leq 10$, our results are compared with those of Biaye et al. [4], of Ivanov et al. [11], of Sakho [20], of Bachau et al. [21] and it can be seen that the present MAOT results agrees well with each other. The small difference between results can be explained by the choice and the character of the trial wavefunction Comparison indicates that for ($Z = 10$) our results at -20,5969 Ry agree very well with them respectively at -20,5609Ry for Sakho [20], -20,52000Ry for [21],-20,6316Ry for .[4] and -20,5265Ry for Ivanov et al .[11]. This good agreement allows us to expect our results with MAOT calculation for 3d^2 ^{1}G doubly excited state up to $Z = 20$ to be accurate.

Table 3 indicates the values of the ξ variational parameter and a comparison of our MAOT results on the calculation of the energies of the singlet doubly excited 4f^2 1I states with other results of [4] [20] and [22] available in the literature. Sakho [20] used the semi-empirical SCUNC method in his work. Similarly, Biaye et al. [4] used the variational method with wave functions of the Hylleraas type. Ho [22] used the complex rotation method in his study.

To our knowledge, there are not yet any experimental data available as well as concerning the H. In general, the comparison shows that our results are in good agreement with the theoretical results of Sakho [20]; of Biaye et al. [4] and Ho [22]. For Z = 10, our MAOT results at 11.56322Ry are in agreement with those provided by Sakho [20] and Biaye [4] respectively at -11.4104Ry and -11.61005Ry. The minimal differences between our MAOT results, SCUNC results of Sakho [20] and variational method results of Biaye [4] can be explained respectively by the choice of a combined wave function (Slater + Hylleraas), the choice of the energy value limited $E\infty$ with a semi-empirical procedure, and the Hylleraas-type wave function.

The good agreement between the results quoted in tables 1-3 indicate the validity of this MAOT variational procedure and his merit to calculate the *(nl^2)* doubly excite state energies.

Table 3: *Variational parameter ξ and total energies E for the $4f^2$ ^1I doubly excited states. The values are reported in Rydberg (Ry). 1Ry= 13.605698 eV.*

Z	Theory				
	ξ	$-E^{MAOT}$	$-E^{Sakho}$	$-E^{Biaye}$	$-E^{Ho}$
1	0.1623	0.04848	-	-	-
2	0.4123	0.32906	0.32380	0.3591	0.34080
3	0.6623	0.85937	0.83464	0.89778	
4	0.9123	1.63938	1.59547	1.68285	
5	1.1623	2.66909	2.60631	2.71550	
6	1.4123	3.95001	3.86714	3.99645	
7	1.6623	5.47766	5.37798	5.52616	
8	1.9123	7.25650	7.13881	7.30493	
9	2.1623	9.28507	9.14965	9.33300	
10	2.4123	11.56332	11.41048	11.61005	
11	2.6623	14.09130			
12	2.9123	16.86898			
13	3.1623	19.89637			
14	3.4123	23.17405			
15	3.6623	26.70029			
16	3.9123	30.47681			
17	4.1623	34.50304			
18	4.4123	38.77898			
19	4.6623	43.30464			
20	4.9123	48.07999			

E^{MAOT}: Energy E of the Modified Atomic Orbital Theory (MAOT), present work; E^{Sakho} [20]; E^{Biaye} [4]; E^{Ho} [22] as quoted in [4].

IV. CONCLUSION

In this work, the variational procedure of the Modified Atomic Orbital Theory (MAOT) has been applied for the calculations energies of the $2p^2$ ^1D, $3d^2$ ^1G, $4f^2$ ^1I Doubly Excited States of Helium isoelectronic sequence from Hydrogen ion H^- to Calcium ion Ca^{18+}. It has demonstrated the possibilities to construct a new correlated wave function adapted to the correct description of the electron-electron correlations phenomena in the (nl^2) doubly excited states of the He-like systems. These very important results obtained in this work indicate the possibility to apply the MAOT variational procedure to the treatment of atomic spectra in two electron systems and probably in more complex atomic systems. The good results give also the possibility to analyze resonance energies via a very

http://dx.doi.org/10.46411/jpsoaphys.2020.02.16

MAOT flexible procedure, in contrast to the complex procedures of experimental and theoretical methods based on the determination of the photoionization cross-section.

ACKNOWLEDGMENTS:

The authors are grateful to the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, and the Orsay Institute of Molecular Sciences (OIMS), University Paris Sud 11, France for support.

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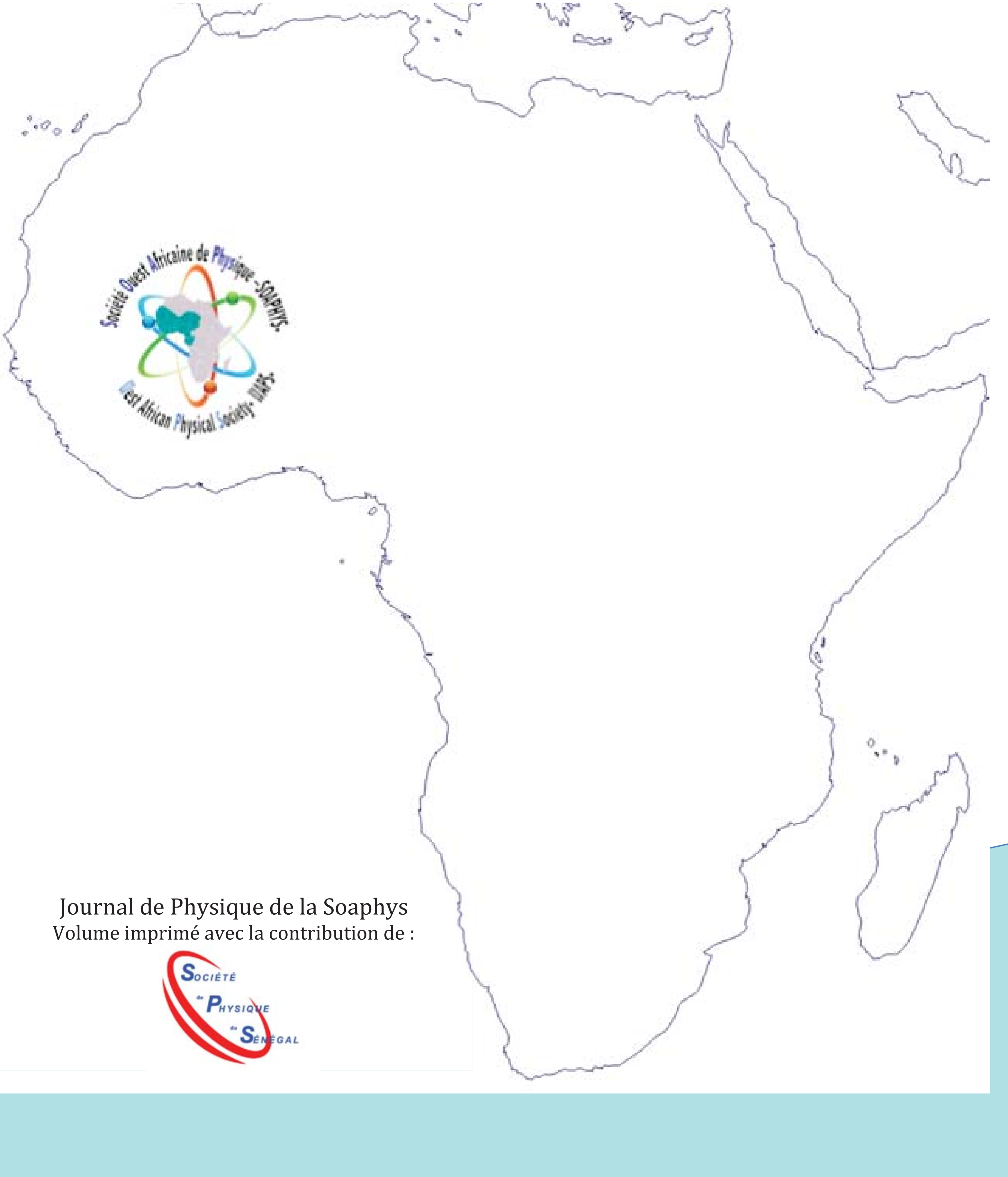

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