

Energy Positions of the $1,3D^e$ Rydberg Series of the He-Like Ions Up to the $N = 9$ Threshold

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How to cite this paper: Dieng M., Diop, B., Sow, M., Gning, Y., Biaye, M., Ndao, A.S. and Wagué, A. (2020) Energy Positions of the $1,3D^e$ Rydberg Series of the He-Like Ions Up to the $N = 9$ Threshold. *Journal of Applied Mathematics and Physics*, 8, 1535-1549.

<https://doi.org/10.4236/jamp.2020.88119>

Received: June 28, 2020

Accepted: August 17, 2020

Published: August 20, 2020

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Abstract

The ${}_n(K, T)_N^{A, 1,3}D_e$ doubly excited states of helium-like ions are investigated using a combination of the no-linear parameters of Hylleraas and the β -parameters of screening constant by unit nuclear charge. Calculations are performed for total energies of low-lying doubly excited states ($N = 2 - 9$) in He-like ions up to $Z = 10$. The results obtained from the novel method are in good agreement with the available theoretical calculations and experimental observations.

Keywords

Electronic Correlations, Variational Calculations, Atoms And Ions, Helium-Like Systems, Singlet States, Triplet States, Matrix Elements, Doubly-Excited States, Autoionization

1. Introduction

The double photoionization of helium has known a considerable importance because of the central role played by the electron-electron correlation in the ejection of two electrons by the absorption of a single photon. Electron-electron correlation is also an essential feature in the process of simultaneous excitation and ionization in which one electron is ejected and residual ion is left in an excited state. At present, we are witnessing a rapid and continuous development work on the study of autoionization states or resonances of atomic systems. Studies of these states resonances in atomic systems have become possible thanks to the development of new experimental methods and high resolving power through

the use of synchrotron sources [1] [2] and lasers [3] in spectroscopic measurements. The study of the properties of atomic systems leads to the development of the theory of atomic processes and allows the development of approximate theoretical methods describing the excitation process. The study of these processes photoabsorption play a very important role in many branches of modern physics; it is necessary to carry out systematic calculations of the main spectroscopic characteristics to push further the development of theoretical methods for the study of these autoionizing states.

The energy positions calculated in the present paper are specified in terms of the supermultiplet classification scheme based on the ${}_n(K, T)_N^{A, 2S+1}L_\pi$ new notation of Herrick [4] as extended and reinterpreted by Lin [5] and replace the traditional $Nlnl'$ notation used in the description of the electron independent model. The observed resonances have been also classified according to the scheme ${}_n\{v\}_N^A$ where $v = 1/2(N - K - T - 1)$ is the vibrational quantum number [6].

In this paper, we present a novel approach to calculate the energy resonances of the ${}^{1,3}D_e$ helium-isoelectronic sequence below the $N = 2 - 9$ ionisation thresholds. We intend to investigate the ${}_n(K, T)_N^{+,-} {}^{1,3}D_e$ doubly excited states energies of helium-like ions. We report total energies for several low-lying and high-lying inter-shell singlet and triplet doubly excited ${}_n(K, T)_N^{+,-} {}^{1,3}D_e$ ($N = 2 - 9$, $n = 3 - 10$) states energies of the helium-like ions up to $Z = 10$. The new procedure used is to combine the variational method with the non-linear parameter of Hylleraas [7] and semi-empirical procedure of Screening Constant by Unit Nuclear Charge (SCUNC) [8].

Section 2, presents the theoretical procedure used in this work.

In Section 3 a presentation and discussion of our calculations along with other theoretical calculations and experimental observations are also made.

2. Theory

2.1. Hamiltonian and Hylleraas-Type Wave Functions

The Hamilton operator for the helium-like ions is written as:

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - \frac{Ze^2}{|\mathbf{r}_1|} - \frac{Ze^2}{|\mathbf{r}_2|} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (1)$$

The vectors \mathbf{r}_1 and \mathbf{r}_2 denote the positions of the two electrons, m the mass of an electron, e the elementary charge and Z the nuclear charge number, Δ_1 and Δ_2 are the Laplace operators of the two electrons, $|\mathbf{r}_1 - \mathbf{r}_2|$ represent the angular part of the wave functions instead of the spherical harmonic in the other Hylleraas type wave functions.

The Schrödinger equation can be written as:

$$H\Phi_{Nlnl'}(\mathbf{r}_1, \mathbf{r}_2) = E\Phi_{Nlnl'}(\mathbf{r}_1, \mathbf{r}_2), \quad (2)$$

$\Phi_{Nlnl'}(\mathbf{r}_1, \mathbf{r}_2)$ represent, the trial non-orthogonal wave functions that we have considered for the description of the inter-shell singlet and triplet doubly excited

states of the helium-like ions. There are special constructions of the incomplete hydrogenic wave functions and Hylleraas type wave functions as follows [7]:

$$\begin{aligned} & \Phi_{Nnl'l'}(\mathbf{r}_1, \mathbf{r}_2) \\ &= \left\langle (2r_1 2r_2)^l \times \sum_{\nu=0}^{\nu=N-l-1} (N^2 r_0^2 \lambda^2 2r_1 2r_2)^\nu + (2r_1 2r_2)^{l'} \times \sum_{\nu'=0}^{\nu'=n-l'-1} (n^2 r_0^2 \lambda'^2 2r_1 2r_2)^{\nu'} \right\rangle (3) \\ & \times (r_1 + r_2)^j (r_1 - r_2)^k |\mathbf{r}_1 - \mathbf{r}_2|^m \exp(\lambda r_1 + \lambda' r_2) \end{aligned}$$

where j, k, m are Hylleraas parameters with $(j, k, m \geq 0)$, λ and λ' are variation parameters;

The wave functions $\varphi_{Nnl'l'}(\mathbf{r}_1, \mathbf{r}_2)$ are not orthogonal;

The set of parameters (j, k, m) define the basis states (*i.e.* the configurations);

The even values of k define the symmetric wave functions describing the singlet states, while the odd values define the antisymmetric wave functions for the triplet states;

N and n denote respectively the principal quantum numbers of the inner and of the outer electron, l and l' are orbital quantum numbers of the two electrons.

The form of the wave functions of the inter-shell singlet and triplet doubly excited state including the correlation effects to the mixing of configurations can be expressed as follows:

$$\Psi_{Nnl'l'}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{jkm} a_{jkm} \Phi_{Nnl'l'} \quad (4)$$

where the set of Hylleraas parameters (j, k, m) defines the basis states (*i.e.* the configurations) and a_{jkm} are the eigenvectors which can be determined by solving the Schrödinger equation:

$$H\Psi_{Nnl'l'}(\mathbf{r}_1, \mathbf{r}_2) = E\Psi_{Nnl'l'}(\mathbf{r}_1, \mathbf{r}_2) \quad (5)$$

The representation of the Schrödinger equation on the non-orthogonal basis (3) leads to the general eigenvalue equation. In what follows, for the sake of brevity we shall denote the triad of Hylleraas parameter (j, k, m) by q .

$$\sum_{q'} (H_{Nnl'l'qq'} - EN_{Nnl'l'qq'}) a_{q'} = 0 \quad (6)$$

with

$$H_{Nnl'l'qq'} = \langle \Psi_{Nnl'l'q}(\mathbf{r}_1, \mathbf{r}_2) | H_{Nnl'l'qq'} | \Psi_{Nnl'l'q'}(\mathbf{r}_1, \mathbf{r}_2) \rangle \quad (7)$$

and

$$N_{Nnl'l'qq'} = \langle \Psi_{Nnl'l'q}(\mathbf{r}_1, \mathbf{r}_2) | \Psi_{Nnl'l'q'}(\mathbf{r}_1, \mathbf{r}_2) \rangle \quad (8)$$

The inter-shell singlet and triplet doubly excited wave functions were found in the basis containing the configurations with the following condition for the Hylleraas parameters $j + k + m \leq 3$, corresponding to the basis dimension $D = 13$ or 7.

In order to obtain the minimum eigenvalue in which we are interested, the calculations are carried out for various values of the parameters λ and λ' .

The eigenvalues E obtained in the present calculations follow the Hylleraas-Undheim theorem [9] and do not include the Feshbach shifts because of the incomplete basis sets.

These calculations have been carried out in the framework of the variational method using interaction basis states with a real Hamiltonian.

According to the Hylleraas-Undheim theorem, a good approximation for the eigenvalues is obtained when the minima of the functions $(d^2(H(\lambda, \lambda'))/d\lambda d\lambda' = 0)$ converge with increasing values of the dimension D and when the functions exhibit a plateau. λ_0 and λ'_0 denotes the values of the λ and λ' -parameters corresponding to the minima of the function and the minimum eigenvalue.

2.2. General Formalism of the SCUNC Method

The screening constant by unit nuclear charge (SCUNC) formalism is used in this work to calculate the energy resonances of the helium-isoelectronic sequence converging to the $N = 2 - 9$ hydrogenic thresholds. In the framework of the SCUNC-method, total energy of $Nnl'^{2S+1}L_\pi$ excited states is expressed in the form (in Ry) [8] [10]:

$$E(Nnl'; {}^{2S+1}L_\pi; Z) = -Z^2 \left\{ \frac{1}{N^2} + \frac{1}{n^2} \left[1 - \beta(Nnl'; {}^{2S+1}L_\pi; Z) \right]^2 \right\} \text{Ry}. \quad (9)$$

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

$$\beta(Nnl'; {}^{2S+1}L_\pi; Z) = \sum_{k=1}^q f_k \left(\frac{1}{Z} \right)^k, \quad (10)$$

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

With the new classification scheme, Equation (9) takes the form (in Ry):

$$E \left[{}_n(K, T)_N^A; {}^{2S+1}L_\pi; Z \right] = -Z^2 \left\{ \frac{1}{N^2} + \frac{1}{n^2} \left[1 - \beta \left[{}_n(K, T)_N^A; {}^{2S+1}L_\pi; Z \right] \right]^2 \right\}, \quad (11)$$

Furthermore, in the framework of the screening constant by unit nuclear charge formalism, the β -screening constant is expressed in terms of λ_0 and λ'_0 who denotes the values of the λ and λ' -variational parameters of Hylleraas corresponding to the minima of the function and the minimum eigenvalue as follows.

$$\begin{aligned} & \beta \left[{}_n(K, T)_N^A; {}^{2S+1}L_\pi; Z, \lambda_0, \lambda'_0 \right] \\ &= \frac{1}{Z^2} \left(\frac{N^2 \lambda_0 + n^2 \lambda'_0}{N^2 + n^2} \right) \left(1 + \frac{L-1}{N+L+S(S+1)} + \frac{L-1}{n+L+S(S+1)} \right) \end{aligned} \quad (12)$$

Using (11), total energy level of an inter-shell ${}_n(K, T)_N^A {}^{2S+1}L_\pi$ doubly excited state in the helium-like ions is given by:

$$E \left[{}_n(K, T)_N^A; {}^{2S+1}L_\pi; Z \right]$$

$$= -(Z - \sigma)^2 \left\{ \frac{1}{N^2} + \frac{1}{n^2} \left[1 - \frac{1}{Z^2} \left(\frac{N^2 \lambda_0 + n^2 \lambda'_0}{N^2 + n^2} \right) \right. \right. \\ \left. \left. \times \left(1 + \frac{L-1}{N+L+S(S+1)} + \frac{L-1}{n+L+S(S+1)} \right) \right]^2 \right\}, \quad (13)$$

where

$$\sigma = \left(48 + \frac{14(N+K+1)(N+K-1) + 14T^2 - 12L(L+1) + 24}{N^2} \right)^{\frac{1}{2}} \quad (14)$$

σ is an effective screening factor or parameter. It is defined to adjust this formula, to accurately describe the resonances parameters for the inter-shell singlet doubly excited states of the helium-like ions.

We use the simple expression (13) to calculate the energy positions of the $^{1,3}D^e$ inter-shell autoionizing states (the two electrons occupy different shells) in helium with an easy calculation program.

3. Results and Discussion

The results of the currently calculations for inter-shell singlet and triplet doubly excited ${}_n(K,T)_N^{+,-} {}^{1,3}D_e$ ($N = 2 - 9$, $n = 3 - 10$) states energies of the helium-like ions up to $Z = 10$ are listed in **Tables 1(a)-(f)** and **Tables 2(a)-(f)**.

In **Table 3**, we have indicated the correspondence between various classification schemes for autoionizing states in two electron systems [4] [5] [6] [11].

Table 4 reports a comparison of the present doubly excited ${}_3(1,0)_2^{+,-} {}^{1,3}D_e$ and ${}_4(1,0)_2^{+,-} {}^{1,3}D_e$ states of helium-like ions with other theoretical results. The present results for ${}_3(1,0)_2^+ {}^1D_e$ match well with those reported by Sakho [8] [10] using a screening constant by unit nuclear charge method (SCUNC), by Ho and Bhatia [12] using a complex-coordinate rotation method (CCR) and by Ivanov and Safronova [13] using a computing double sum (CDS). For ${}_4(1,0)_2^+ {}^1D_e$ levels of the series, the present results agree well with the SCUNC results of Sakho [8] [10] and the CDS results of Ivanov and Safronova [13]. ${}_3(1,0)_2^- {}^3D_e$ levels of up to $Z = 10$ are reported by Sakho [8] [10] using a SCUNC method, by Ho and Bhatia [12] using CCR and by Ivanov and Safronova [13] a CDS method and, in general, they are close to our results. For ${}_4(1,0)_2^- {}^3D_e$ levels of the series, our results agree well with the results of Sakho [8] [10] and those of Ivanov and Safronova [13].

In **Table 5**, we present a comparison of the present doubly excited ${}_3(1,0)_2^+ {}^1D_e$ and ${}_4(1,0)_2^+ {}^1D_e$ states of helium-like ions with other theoretical and experimental results. Eiglsperger *et al.* [14], use a spectral method (SM), Chen [15] using a saddle-point complex rotation method (SPCR), Oza [16] using a close-coupling method (CC) and Lipsky *et al.* [17] using a truncated diagonalization method (TDM) and above the present results. Our results is also quite close to the experimental observations of Hicks and Comer [18] using a Ejected Electron Spectroscopy (EES). The comparison of our calculated energies, with

Table 1. (a) Energy resonances of doubly excited ${}_n(K,T)_2^+ {}^1D_e$ ($n = 3 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (b) Energy resonances of doubly excited ${}_n(K,T)_3^+ {}^1D_e$ ($n = 4 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (c) Energy resonances of doubly excited ${}_n(K,T)_4^+ {}^1D_e$ ($n = 3 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (d) Energy resonances of doubly excited ${}_n(K,T)_5^+ {}^1D_e$ ($n = 6 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (e) Energy resonances of doubly excited ${}_n(K,T)_6^+ {}^1D_e$ ($n = 7 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (f) Energy resonances of doubly excited ${}_n(K,T)_7^+ {}^1D_e$ ($n = 8 - 10$), ${}_n(K,T)_8^+ {}^1D_e$ ($n = 9, 10$) and ${}_{10}(K,T)_9^+ {}^1D_e$ states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV.

(a)									
${}_n(K,T)_N^A$	${}_3(1,0)_2^+$	${}_4(1,0)_2^+$	${}_5(1,0)_2^+$	${}_6(1,0)_2^+$	${}_7(1,0)_2^+$	${}_8(1,0)_2^+$	${}_9(1,0)_2^+$	${}_{10}(1,0)_2^+$	
${}_n(\nu)_N^+$	${}_3(0)_2^+$	${}_4(0)_2^+$	${}_5(0)_2^+$	${}_6(0)_2^+$	${}_7(0)_2^+$	${}_8(0)_2^+$	${}_9(0)_2^+$	${}_{10}(0)_2^+$	
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	1.137948	1.098295	1.052718	1.035273	1.023773	1.016707	1.011929	1.008409	
3	2.749137	2.569488	2.437033	2.378202	2.340952	2.317493	2.301526	2.289922	
4	5.082443	4.665643	4.401318	4.276665	4.198931	4.149518	4.115806	4.091428	
5	8.137928	7.386781	6.945591	6.730676	6.597722	6.512788	6.454775	6.412931	
6	11.915616	10.732912	10.069858	9.740238	9.537325	9.407306	9.318432	9.254432	
7	16.415513	14.704038	13.774121	13.305354	13.017743	12.833072	12.706780	12.615933	
8	21.637625	19.300162	18.058381	17.426023	17.038976	16.790088	16.619819	16.497433	
9	27.581954	24.521283	22.922641	22.102248	21.601025	21.278353	21.057549	20.898933	
10	34.248502	30.367404	28.366899	27.334027	26.703890	26.297868	26.019970	25.820433	

(b)							
${}_n(K,T)_N^A$	${}_4(1,1)_3^+$	${}_5(1,1)_3^+$	${}_6(1,1)_3^+$	${}_7(1,1)_3^+$	${}_8(1,1)_3^+$	${}_9(1,1)_3^+$	${}_{10}(1,1)_3^+$
${}_n(\nu)_N^+$	${}_4(0)_3^+$	${}_5(0)_3^+$	${}_6(0)_3^+$	${}_7(0)_3^+$	${}_8(0)_3^+$	${}_9(0)_3^+$	${}_{10}(0)_3^+$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.575269	0.516417	0.492580	0.478029	0.469301	0.463554	0.459439
3	1.374520	1.219820	1.149648	1.107017	1.080598	1.062900	1.050233
4	2.520974	2.225428	2.084482	1.999035	1.945361	1.909154	1.883245
5	4.014643	3.533251	3.297088	3.154088	3.063592	3.002319	2.958477
6	5.855531	5.143293	4.787470	4.572178	4.435294	4.342397	4.275931
7	8.043639	7.055556	6.555628	6.253304	6.060468	5.929387	5.835606
8	10.578968	9.270040	8.601564	8.197469	7.939114	7.763291	7.637503
9	13.461518	11.786745	10.925276	10.404672	10.071231	9.844108	9.681622
10	16.691290	14.605672	13.526766	12.874913	12.456820	12.171838	11.967963

(c)

${}_n(K, T)_N^A$	${}_5(1, 2)_4^+$	${}_6(1, 2)_4^+$	${}_7(1, 2)_4^+$	${}_8(1, 2)_4^+$	${}_9(1, 2)_4^+$	${}_{10}(1, 2)_4^+$
${}_n(v)_N^+$	${}_5(0)_4^+$	${}_6(0)_4^+$	${}_7(0)_4^+$	${}_8(0)_4^+$	${}_9(0)_4^+$	${}_{10}(0)_4^+$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.329096	0.303092	0.287370	0.277886	0.271657	0.267232
3	0.794282	0.720412	0.675786	0.648057	0.629518	0.616310
4	1.464456	1.318278	1.230010	1.174472	1.137065	1.110385
5	2.339624	2.096696	1.950048	1.857135	1.794303	1.749458
6	3.419790	3.055667	2.835901	2.696047	2.601230	2.533530
7	4.704954	4.195193	3.887569	3.691208	3.557849	3.462602
8	6.195118	5.515274	5.105053	4.842618	4.664158	4.536673
9	7.890281	7.015910	6.488353	6.150278	5.920159	5.755745
10	9.790443	8.697102	8.037469	7.614188	7.325850	7.119816

(d)

${}_n(K, T)_N^A$	${}_6(1, 3)_5^+$	${}_7(1, 3)_5^+$	${}_8(1, 3)_5^+$	${}_9(1, 3)_5^+$	${}_{10}(1, 3)_5^+$
${}_n(v)_N^+$	${}_6(0)_5^+$	${}_7(0)_5^+$	${}_8(0)_5^+$	${}_9(0)_5^+$	${}_{10}(0)_5^+$
Z	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.211285	0.196862	0.187933	0.181967	0.177684
3	0.514678	0.472280	0.445510	0.427427	0.414466
4	0.953617	0.868506	0.814331	0.777575	0.751244
5	1.528108	1.385546	1.294401	1.232412	1.188021
6	2.238152	2.023401	1.885718	1.791939	1.724797
7	3.083751	2.782071	2.588286	2.456157	2.361573
8	4.064904	3.661557	3.402102	3.225066	3.098348
9	5.181613	4.661858	4.327169	4.098666	3.935123
10	6.433876	5.782976	5.363485	5.076958	4.871898

(e)

${}_n(K, T)_N^A$	${}_7(1, 4)_6^+$	${}_8(1, 4)_6^+$	${}_9(1, 4)_6^+$	${}_{10}(1, 4)_6^+$
${}_n(v)_N^+$	${}_7(0)_6^+$	${}_8(0)_6^+$	${}_9(0)_6^+$	${}_{10}(0)_6^+$
Z	$-E$	$-E$	$-E$	$-E$
2	0.148522	0.139600	0.133600	0.129286
3	0.363168	0.336410	0.318268	0.305251
4	0.674177	0.620019	0.583178	0.556768
5	1.081556	0.990432	0.928333	0.883840
6	1.585306	1.447649	1.353734	1.286466
7	2.185426	1.991671	1.859381	1.764647
8	2.881918	2.622499	2.445275	2.318384
9	3.674781	3.340131	3.111416	2.947676
10	4.564016	4.144569	3.857804	3.652524

(f)

${}_n(K,T)_N^A$	${}_8(1,5)_7^+$	${}_9(1,5)_7^+$	${}_{10}(1,5)_7^+$	${}_9(1,6)_8^+$	${}_{10}(1,6)_8^+$	${}_{10}(1,7)_9^+$
${}_n(\nu)_N^+$	${}_8(0)_7^+$	${}_9(0)_7^+$	${}_{10}(0)_7^+$	${}_9(0)_8^+$	${}_{10}(0)_8^+$	${}_{10}(0)_9^+$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.110260	0.104308	0.100017	0.085390	0.081088	0.068174
3	0.270285	0.252226	0.239250	0.209526	0.196530	0.167351
4	0.502371	0.465647	0.439296	0.389598	0.363219	0.311216
5	0.806521	0.744575	0.700157	0.625611	0.581157	0.499771
6	1.182736	1.089009	1.021833	0.917564	0.850343	0.733017
7	1.631017	1.498950	1.404326	1.265457	1.170780	1.010954
8	2.151364	1.974399	1.847634	1.669292	1.542466	1.333582
9	2.743777	2.515355	2.351759	2.129068	1.965402	1.700901
10	3.408256	3.121819	2.916700	2.644785	2.439588	2.112912

Table 2. (a) Energy resonances of doubly excited ${}_n(K,T)_2^{-3}D_e$ ($n = 3 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (b) Energy resonances of doubly excited ${}_n(K,T)_3^{-3}D_e$ ($n = 4 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (c) Energy resonances of doubly excited ${}_n(K,T)_4^{-3}D_e$ ($n = 5 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (d) Energy resonances of doubly excited ${}_n(K,T)_5^{-3}D_e$ ($n = 6 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (e) Energy resonances of doubly excited ${}_n(K,T)_6^{-3}D_e$ ($n = 7 - 10$) states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV. (f) Energy resonances of doubly excited ${}_n(K,T)_7^{-3}D_e$ ($n = 8 - 10$), ${}_n(K,T)_8^{-1}D_e$ ($n = 9, 10$) and ${}_{10}(K,T)_9^{-1}D_e$ states of helium-like ions ($Z = 2 - 10$). The results are expressed in Rydberg units: 1 Ry = 13.6056925 eV.

(a)

${}_n(K,T)_N^A$	${}_3(1,0)_2^-$	${}_4(1,0)_2^-$	${}_5(1,0)_2^-$	${}_6(1,0)_2^-$	${}_7(1,0)_2^-$	${}_8(1,0)_2^-$	${}_9(1,0)_2^-$	${}_{10}(1,0)_2^-$
${}_n(\nu)_N^-$	${}_3(0)_2^-$	${}_4(0)_2^-$	${}_5(0)_2^-$	${}_6(0)_2^-$	${}_7(0)_2^-$	${}_8(0)_2^-$	${}_9(0)_2^-$	${}_{10}(0)_2^-$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	1.168691	1.117142	1.067396	1.047609	1.034798	1.026906	1.021578	1.017679
3	2.803615	2.600772	2.461239	2.398119	2.358504	2.333539	2.316567	2.304271
4	5.160762	4.709403	4.435082	4.304185	4.223027	4.171422	4.136248	4.110864
5	8.240131	7.443033	6.988925	6.765806	6.628366	6.540555	6.480620	6.437457
6	12.041722	10.801663	10.122768	9.782983	9.574521	9.440938	9.349683	9.284049
7	16.565536	14.785294	13.836611	13.355715	13.061492	12.872571	12.743438	12.650642
8	21.811572	19.393924	18.130454	17.484003	17.089280	16.835454	16.661884	16.537235
9	27.779829	24.627555	23.004297	22.167847	21.657884	21.329587	21.105022	20.943827
10	34.470310	30.486185	28.458140	27.407246	26.767305	26.354970	26.072850	25.870420

(b)

${}_n(K, T)_N^A$	${}_4(1, 1)_3^-$	${}_5(1, 1)_3^-$	${}_6(1, 1)_3^-$	${}_7(1, 1)_3^-$	${}_8(1, 1)_3^-$	${}_9(1, 1)_3^-$	${}_{10}(1, 1)_3^-$
${}_n(v)_N^-$	${}_4(0)_3^-$	${}_5(0)_3^-$	${}_6(0)_3^-$	${}_7(0)_3^-$	${}_8(0)_3^-$	${}_9(0)_3^-$	${}_{10}(0)_3^-$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.584259	0.523515	0.498319	0.482969	0.473712	0.467603	0.463233
3	1.389275	1.231549	1.159022	1.115012	1.087662	1.069322	1.056203
4	2.541512	2.241805	2.097503	2.010093	1.955084	1.917954	1.891396
5	4.040971	3.554283	3.313761	3.168213	3.075979	3.013500	2.968811
6	5.887653	5.168984	4.807798	4.589372	4.450346	4.355960	4.288448
7	8.081557	7.085907	6.579612	6.273569	6.078185	5.945333	5.850307
8	10.622683	9.305052	8.629204	8.220804	7.959496	7.781620	7.654388
9	13.511032	11.826419	10.956573	10.431079	10.094280	9.864821	9.700692
10	16.746603	14.650009	13.561721	12.904391	12.482536	12.194935	11.989218

(c)

${}_n(K, T)_N^A$	${}_5(1, 2)_4^-$	${}_6(1, 2)_4^-$	${}_7(1, 2)_4^-$	${}_8(1, 2)_4^-$	${}_9(1, 2)_4^-$	${}_{10}(1, 2)_4^-$
${}_n(v)_N^-$	${}_5(0)_4^-$	${}_6(0)_4^-$	${}_7(0)_4^-$	${}_8(0)_4^-$	${}_9(0)_4^-$	${}_{10}(0)_4^-$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.334719	0.307264	0.290734	0.280741	0.274176	0.269521
3	0.803646	0.727309	0.681307	0.652700	0.633575	0.619965
4	1.477573	1.327909	1.237696	1.180908	1.142665	1.115409
5	2.356500	2.109065	1.959902	1.865366	1.801446	1.755853
6	3.440426	3.070776	2.847924	2.706075	2.609919	2.541297
7	4.729353	4.213043	3.901763	3.703033	3.568083	3.471741
8	6.223280	5.535865	5.121418	4.856241	4.675938	4.547184
9	7.922207	7.039243	6.506889	6.165700	5.933485	5.767628
10	9.826133	8.723176	8.058176	7.631408	7.340723	7.133072

(d)

${}_n(K, T)_N^A$	${}_6(1, 3)_5^-$	${}_7(1, 3)_5^-$	${}_8(1, 3)_5^-$	${}_9(1, 3)_5^-$	${}_{10}(1, 3)_5^-$
${}_n(v)_N^-$	${}_6(0)_5^-$	${}_7(0)_5^-$	${}_8(0)_5^-$	${}_9(0)_5^-$	${}_{10}(0)_5^-$
Z	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.214612	0.199431	0.190039	0.183773	0.179287
3	0.520288	0.476574	0.448993	0.430382	0.417063
4	0.961519	0.874534	0.819198	0.781683	0.754839
5	1.538305	1.393310	1.300653	1.237675	1.192615
6	2.250647	2.032902	1.893357	1.798358	1.730391
7	3.098545	2.793311	2.597312	2.463733	2.368167
8	4.081998	3.674536	3.412516	3.233799	3.105943
9	5.201007	4.676577	4.338971	4.108557	3.943719
10	6.455572	5.799434	5.376676	5.088006	4.881495

(e)				
${}_n(K, T)_N^A$	${}_7(1, 4)_6^-$	${}_8(1, 4)_6^-$	${}_9(1, 4)_6^-$	${}_{10}(1, 4)_6^-$
${}_n(\nu)_N^-$	${}_7(0)_6^-$	${}_8(0)_6^-$	${}_9(0)_6^-$	${}_{10}(0)_6^-$
Z	$-E$	$-E$	$-E$	$-E$
2	0.150622	0.141277	0.135007	0.130510
3	0.366712	0.339212	0.320593	0.307256
4	0.679174	0.623953	0.586426	0.559557
5	1.088007	0.995499	0.932506	0.887414
6	1.593213	1.453851	1.358834	1.290826
7	2.194790	1.999008	1.865408	1.769794
8	2.892739	2.630971	2.452229	2.324317
9	3.687060	3.349740	3.119296	2.954396
10	4.577753	4.155314	3.866611	3.660030

(f)						
${}_n(K, T)_N^A$	${}_8(1, 5)_7^-$	${}_9(1, 5)_7^-$	${}_{10}(1, 5)_7^-$	${}_9(1, 6)_8^-$	${}_{10}(1, 6)_8^-$	${}_{10}(1, 7)_9^-$
${}_n(\nu)_N^-$	${}_8(0)_7^-$	${}_9(0)_7^-$	${}_{10}(0)_7^-$	${}_9(0)_8^-$	${}_{10}(0)_8^-$	${}_{10}(0)_9^-$
Z	$-E$	$-E$	$-E$	$-E$	$-E$	$-E$
2	0.111671	0.105468	0.101010	0.086385	0.081927	0.068904
3	0.272666	0.254164	0.240892	0.211200	0.197929	0.168576
4	0.505728	0.468367	0.441591	0.391956	0.365180	0.312940
5	0.810856	0.748077	0.703105	0.628654	0.583682	0.501995
6	1.188050	1.093296	1.025436	0.921293	0.853433	0.735741
7	1.637311	1.504022	1.408584	1.269874	1.174435	1.014179
8	2.158637	1.980256	1.852547	1.674395	1.546687	1.337308
9	2.752031	2.521997	2.357327	2.134859	1.970188	1.705128
10	3.417490	3.129246	2.922923	2.651263	2.444940	2.117640

Table 3. Correspondence between various classification schemes for autoionizing states in two-electron systems below the $N = 2 - 9$ hydrogenic threshold. $(2S + 1)$ is the multiplicity where S denotes the total spin angular momentum, L is the total orbital angular momentum, π represents the parity, N and n are respectively the principal quantum numbers of the inner and the outer electron. S , L , π , N and n are common to all the schemes. The correlation quantum numbers K , T and A used to label each state are introduced to complete the description.

<i>Usual Classification</i> $Nlnl'^{2S+1}L^{\pi}$	<i>Conneely and Lipsky</i> (N, n, a)	<i>Herrick and Sinanoglu</i> ${}_n(K, T)_N$	<i>Sadeghpour</i> ${}_n(\nu)_N$	<i>Lin</i> A	<i>Lowest N of the series</i>
$2pnp^1D_e$	$(2, n, a)$	${}_n(1, 0)_2$	${}_n(0)_2$	+	2
$2pnp^3D_e$	$(2, n, a)$	${}_n(1, 0)_2$	${}_n(0)_2$	-	2
$3pnp^1D_e$	$(3, n, a)$	${}_n(1, 1)_3$	${}_n(0)_3$	+	3
$3pnp^3D_e$	$(3, n, a)$	${}_n(1, 1)_3$	${}_n(0)_3$	-	3
$4pnp^1D_e$	$(4, n, a)$	${}_n(1, 2)_4$	${}_n(0)_4$	+	4

Continued

$4pnp\ ^3D_e$	$(4, n, a)$	${}_n(1, 2)_4$	${}_n(0)_4$	-	4
$5pnp\ ^1D_e$	$(5, n, a)$	${}_n(1, 3)_5$	${}_n(0)_5$	+	5
$5pnp\ ^3D_e$	$(5, n, a)$	${}_n(1, 3)_5$	${}_n(0)_5$	-	5
$6pnp\ ^1D_e$	$(6, n, a)$	${}_n(1, 4)_6$	${}_n(0)_6$	+	6
$6pnp\ ^3D_e$	$(6, n, a)$	${}_n(1, 4)_6$	${}_n(0)_6$	-	6
$7pnp\ ^1D_e$	$(7, n, a)$	${}_n(1, 5)_7$	${}_n(0)_7$	+	7
$7pnp\ ^3D_e$	$(7, n, a)$	${}_n(1, 5)_7$	${}_n(0)_7$	-	7
$8pnp\ ^1D_e$	$(8, n, a)$	${}_n(1, 6)_8$	${}_n(0)_8$	+	8
$8pnp\ ^3D_e$	$(8, n, a)$	${}_n(1, 6)_8$	${}_n(0)_8$	-	8
$9pnp\ ^1D_e$	$(9, n, a)$	${}_n(1, 7)_9$	${}_n(0)_9$	+	9
$9pnp\ ^3D_e$	$(9, n, a)$	${}_n(1, 7)_9$	${}_n(0)_9$	-	9

Table 4. Comparison of the present doubly excited ${}_3(1,0)_2^{+,-1,3}D_e$ and ${}_4(1,0)_2^{+,-1,3}D_e$ states of helium-like ions with other theoretical results. SCUNC: screening constant by unit nuclear charge method, CCR: complex-coordinate rotation method, CDS: computing double sum. The energy resonances ($-E$) are expressed in Rydberg units.

${}_n(K, T)_N^A$	${}_3(1,0)_2^+$				${}_4(1,0)_2^+$		
${}_n(0)_N^+$	${}_3(0)_2^+$				${}_4(0)_2^+$		
Z	Present	SCUNC	CCR	CDS	Present	SCUNC	CDS
2	1.137948	1.138140	1.138441	1.143860	1.098295	1.072900	1.069020
3	2.749137	2.747800	2.748201	2.738740	2.569488	2.520640	2.513040
4	5.082443	5.079840	5.080575	5.055840	4.665643	4.593440	4.582080
5	8.137928	8.134160	8.135532	8.095160	7.386781	7.291240	7.276100
6	11.915616	11.910740	11.912922	11.856700	10.732912	10.614060	10.595140
7	16.415513	16.409560	16.412662	16.340460	14.704038	14.561900	14.539160
8	21.637625	21.630620	21.634700	21.546440	19.300162	19.134720	19.108200
9	27.581954	27.573900	27.579020	27.474640	24.521283	24.332560	24.302220
10	34.248502	34.239420	34.245600	34.125080	30.367404	30.155400	30.121260
${}_n(K, T)_N^A$	${}_3(1,0)_2^-$				${}_4(1,0)_2^-$		
${}_n(0)_N^-$	${}_3(0)_2^-$				${}_4(0)_2^-$		
Z	Present	SCUNC	CCR	CDS	Present	SCUNC	CDS
2	1.168691	1.166740	1.167568	1.157920	1.117142	1.081500	1.079220
3	2.803615	2.807060	2.811136	2.794240	2.600772	2.541340	2.536540
4	5.160762	5.170820	5.176675	5.152780	4.709403	4.627100	4.618860
5	8.240131	8.257280	8.264268	8.233540	7.443033	7.338220	7.326160
6	12.041722	12.066200	12.073986	12.036540	10.801663	10.674520	10.658480
7	16.565536	16.597480	16.605864	16.561740	14.785294	14.635940	14.615800
8	21.811572	21.851060	21.859925	21.809180	19.393924	19.222400	19.198120
9	27.779829	27.826920	27.836179	27.778820	24.627555	24.433920	24.405420
10	34.470310	34.525040	34.534636	34.470700	30.486185	30.270460	30.237740

Table 5. Comparison of the present doubly excited ${}_n(1,0)_2^+ {}^1D_e$ ($n = 3 - 10$) and ${}_n(1,1)_3^+ {}^1D_e$ ($n = 4 - 10$) states of helium-like ions with other theoretical results. SM: spectral method, SPCR: saddle-point complex-rotation method, CC: close-coupling method, TDM: truncated diagonalization method, EES: ejected electron spectroscopy, CIM: Configuration Interaction Method. The energy resonances ($-E$) are expressed in Rydberg units.

${}_n(K,T)_N^A$	${}_n(0)_N^+$	Present	SM	SPCR	CC	TDM	EES	CIM
${}_3(1,0)_2^+$	${}_3(0)_2^+$	1.137948	1.138432	1.138386	1.138220	1.135406	1.139964	1.138738
${}_4(1,0)_2^+$	${}_4(0)_2^+$	1.098295	1.073449	1.073430	1.073380	1.072080	1.074550	1.073570
${}_5(1,0)_2^+$	${}_5(0)_2^+$	1.052718	1.045483	1.045474	1.045440	1.044778		1.045542
${}_6(1,0)_2^+$	${}_6(0)_2^+$	1.035273	1.030908	1.030902	1.030880	1.030502		1.030940
${}_7(1,0)_2^+$	${}_7(0)_2^+$	1.023773	1.022360	1.022356	1.022240			
${}_8(1,0)_2^+$	${}_8(0)_2^+$	1.016707	1.016923	1.016998	1.016540			
${}_9(1,0)_2^+$	${}_9(0)_2^+$	1.011929	1.013252					
${}_{10}(1,0)_2^+$	${}_{10}(0)_2^+$	1.008409	1.010657					
${}_4(1,1)_3^+$	${}_4(0)_3^+$	0.575269	0.551730			0.552072		
${}_5(1,1)_3^+$	${}_5(0)_3^+$	0.516417	0.506676			0.509076		
${}_6(1,1)_3^+$	${}_6(0)_3^+$	0.492580	0.484738			0.484648		
${}_7(1,1)_3^+$	${}_7(0)_3^+$	0.478029	0.470936			0.470846		
${}_8(1,1)_3^+$	${}_8(0)_3^+$	0.469301	0.464014					
${}_9(1,1)_3^+$	${}_9(0)_3^+$	0.463554	0.459494					
${}_{10}(1,1)_3^+$	${}_{10}(0)_3^+$	0.459439	0.456380					

the very precise and recent values calculated by Restrepo [19] using the configuration interaction method (CIM), is very reasonable.

In **Table 6**, the results obtained for ${}_n(1,0)_2^- {}^3D_e$ and ${}_n(1,1)_2^- {}^3D_e$ resonances in the helium-like ions are displayed and compared with the data of Eiglsperger *et al.* [14], Argenti [20] using a B-spline K-matrix method (BKM), Chen [15], Lipsky *et al.* [17] and Cuartas and Vicario [19]. It can be seen that, the present calculations agree well with those of the cited authors.

4. Summary

In this work, we present an extensive analysis of the inter-shell singlet and triplet doubly excited ${}_n(K,T)_N^{+,-} {}^{1,3}D_e$ ($N = 2 - 9$, $n = 3 - 10$) states energies of the helium-like ions up to $Z = 10$ using a simple approach. The calculations have been done by using the variational method with the no-linear parameters of Hylleraas and the β -parameters of screening constant by unit nuclear charge. We have used a simple equation (13) to calculate resonance parameters for inter-shell ${}^{1,3}D_e$ autoionizing states in helium (the two electrons occupy the different shells).

Comparisons with other theoretical calculations and experimental observations are in good agreement. For some states, we have noticed small differences

Table 6. Comparison of the present doubly excited ${}_n(1,0)_2^{-3}D_e$ ($n = 3-10$) and ${}_n(1,1)_3^{-3}D_e$ ($n = 4 - 10$) states of helium-like ions with other theoretical results. SM: Spectral Method, BKM: B-spline K-matrix method, SPCR: Saddle-Point Complex-Rotation method, TDM: Truncated Diagonalization Method, CIM: Configuration Interaction Method. The energy resonances ($-E$) are expressed in Rydberg units.

${}_n(K,T)_N^A$	${}_n(0)_N^-$	Present	SM	BKM	SPCR	TDM	CIM
${}_3(1,0)_2^-$	${}_3(0)_2^-$	1.168691	1.167568	1.167568	1.167568	1.166390	1.167590
${}_4(1,0)_2^-$	${}_4(0)_2^-$	1.117142	1.083357	1.083357	1.083358	1.082742	1.083362
${}_5(1,0)_2^-$	${}_5(0)_2^-$	1.067396	1.050037	1.050037	1.050036	1.049710	1.050038
${}_6(1,0)_2^-$	${}_6(0)_2^-$	1.047609	1.033377	1.033376	1.033374	1.033188	1.033376
${}_7(1,0)_2^-$	${}_7(0)_2^-$	1.034798	1.023849	1.023848		1.023732	
${}_8(1,0)_2^-$	${}_8(0)_2^-$	1.026906	1.017890	1.017889			
${}_9(1,0)_2^-$	${}_9(0)_2^-$	1.021578	1.013915	1.013915			
${}_{10}(1,0)_2^-$	${}_{10}(0)_2^-$	1.017679	1.011132	1.011132			
${}_4(1,1)_3^-$	${}_4(0)_3^-$	0.584259	0.566093	0.566092		0.565924	
${}_5(1,1)_3^-$	${}_5(0)_3^-$	0.523515	0.511859	0.511858		0.511666	
${}_6(1,1)_3^-$	${}_6(0)_3^-$	0.498319	0.487148	0.487146		0.486994	
${}_7(1,1)_3^-$	${}_7(0)_3^-$	0.482969	0.473854	0.473850		0.473758	
${}_8(1,1)_3^-$	${}_8(0)_3^-$	0.473712	0.465907	0.465905			
${}_9(1,1)_3^-$	${}_9(0)_3^-$	0.467603	0.460788	0.460786			
${}_{10}(1,1)_3^-$	${}_{10}(0)_3^-$	0.463233	0.457300	0.457299			

between our results and other data, which are due to the approximations in the calculation of the variational parameters.

The prospect of this work is to improve our calculation method by modifying the parameters, to have a very good convergence of results. In this case, it will be possible to study the ${}^1,3F^o$, ${}^1,3G^e$ and other states energies of Helium-Like Ions.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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