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Doubly excited $^{1,3}P^o$ resonances of helium below the $N=2$–9 ionisation thresholds

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HIGHTLIGHTS

- A simple approach, to calculate inter-shell ${}_n(K,T)_N^{A\,1,3}P_o$ states.
- The calculations use two methods combined.
- A simple expression is used to calculate intershell $^{1,3}P^o$ states.
- Satisfactory agreements between theoretical and experimental literature values up to $Z=10$.

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ABSTRACT

A novel approach is used to evaluate energies of singlet and triplet resonance states of helium below the $N=2$–9 hydrogenic thresholds. We have combined the variational method with the no-linear parameters of Hylleraas and the β-parameters of screening constant by unit nuclear charge. Comparison with various available theoretical and experimental literature values indicates a good agreement.

1. Introduction

Nowadays, the studies of the electromagnetic interaction of atoms and ions with light have shown the importance of electronic correlation effects in the photoionization processes. The first experiments on the autoionization resonance started with the works of Madden and Codling (1963, 1965) who studied by means of a synchrotron radiation source, the helium photoabsorption spectra and shed light to several resonances in the spectral zone of the ultraviolet rays distant. The process on the studies of photoabsorption and photoionization of atoms and ions plays an important role and has shown a significant advance with the use of synchrotron radiation sources in spectroscopy experiments (Elving and Winefordner, 1979; Eland, 1984; Letokhov, 1987).

The present work is an extension of the earlier calculations for inter-shell ${}_n(K,T)_N^{A\,1,3}P_o$ doubly excited states energies of helium-like ions. We have combined the variational method with the non-linear parameter of Hylleraas (Biaye et al., 2009; Dieng et al., 2010) and semi-empirical procedure of Screening Constant by Unit Nuclear Charge (SCUNC) (Sakho et al., 2010; Sakho, 2011a, 2011b). And we have calculated some low-lying and high-lying inter-shell singlet and triplet doubly excited $N\,ln\,l'$ (with $N=2-9$, $n=3-10$) states energies of the helium-like ions with $Z=2-10$.

Section 2 presents the theoretical procedure used in this work.

In Section 3 the comparisons of our results with other calculations and experimental data are made.

2. Theory

2.1. Hamiltonian and Hylleraas-type wave functions

The Schrödinger equation for the helium-like ions can be written as

$$H\,\Phi_{N\,\mathrm{ln}\,l'}(\vec{r}_1,\ \vec{r}_2)=E\,\Phi_{N\,\mathrm{ln}\,l'}(\vec{r}_1,\ \vec{r}_2), \tag{1}$$

where H is the Hamiltonian of the helium-like ions, r_1 and r_2 are the coordinates of the electrons, $\Phi_{Nnl'}(\vec{r}_1,\ \vec{r}_2)$ represent, the trial non-orthogonal wave functions that we have considered for the description of the inter-shell singlet and triplet doubly

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excited states of the helium-like ions. There are special constructions of the incomplete hydrogenic wave functions and Hylleraas type wave functions as follows (Biaye et al., 2009; Dieng et al., 2010):

$$\Phi_{Nlnl'}(\vec{r}_1, \vec{r}_2) = \langle (2r_1 2r_2)^l \times \sum_{\nu=0}^{\nu=N-l-1} (N^2 r_0^2 \lambda^2 2r_1 2r_2)^{\nu} + (2r_1 2r_2)^{l'} \times \sum_{\nu'=0}^{\nu'=n-l'-1} (n^2 r_0^2 \lambda'^2 2r_1 2r_2)^{\nu'} \rangle \times (r_1+r_2)^j (r_1-r_2)^k |\vec{r}_1 - \vec{r}_2|^m \exp(\lambda r_1 + \lambda' r_2) \quad (2)$$

where j, k, m are Hylleraas parameters with (j, k, $m \geq 0$), λ and λ' are variation parameters,
the wave functions $\varphi_{Nlnl'}(\vec{r}_1, \vec{r}_2)$ 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 are the principal quantum numbers; l and $l'$are orbital quantum numbers.
$|\vec{r}_1, \vec{r}_2|$, represent the angular part of the wave functions instead of the spherical harmonic in the other Hylleraas type wave functions.

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:

$$\Psi_{N\,\mathrm{ln}\,l'}(\vec{r}_1, \vec{r}_2) = \sum_{jkm} a_{jkm} \Phi_{N\,\mathrm{ln}\,l'}, \quad (3)$$

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:

$$H\,\Psi_{N\,\mathrm{ln}\,l'}(\vec{r}_1, \vec{r}_2) = E\,\Psi_{N\,\mathrm{ln}\,l'}(\vec{r}_1, \vec{r}_2), \quad (4)$$

In what follows, for the sake of brevity we shall denote the triad of Hylleraas parameter (j ,k, m) by q.

$$\sum_{q'} (H_{N\,\mathrm{ln}\,l'qq'} - E\,N_{N\,\mathrm{ln}\,l'qq'}) a_{q'} = 0 \quad (5)$$

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 (Hylleraas and Undheim, 1930) 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 $Nlnl'^{2S+1}L_\pi$ excited states is expressed in the form (in Ry) (Sakho, 2011a, 2011b.):

$$E(Nlnl';\ ^{2S+1}L_\pi;\ Z) = -Z^2 \left\{ \frac{1}{N^2} + \frac{1}{n^2}[1-\beta(Nlnl';\ ^{2S+1}L_\pi;\ Z)]^2 \right\} \mathrm{Ry}. \quad (6)$$

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:

$$\beta(Nlnl';\ ^{2S+1}L_\pi;\ Z) = = \sum_{k=1}^{q} f_k \left(\frac{1}{Z}\right)^k, \quad (7)$$

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

With the new classification scheme, Eq. (6) takes the form (in Ry):

$$E[_n(K,\ T)^A_N;\ ^{2S+1}L_\pi;\ Z] = -Z^2 \left\{ \frac{1}{N^2} + \frac{1}{n^2}[1-\beta[_n(K,\ T)^A_N;\ ^{2S+1}L_\pi;\ Z]]^2 \right\}, \quad (8)$$

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:

$$\beta[_n(K,\ T)^A_N;\ ^{2S+1}L_\pi;\ Z,\ \lambda_0,\ \lambda'_0] = \frac{1}{Z^2}\left(\frac{N^2\lambda_0 + n^2\lambda'_0}{N^2+n^2}\right)\left(1 + \frac{L+1}{N+L+S(S+1)} + \frac{L+1}{n+L+S(S+1)}\right) \quad (9)$$

Table 1
Energy resonances of doubly excited $_n(0,1)_2^{+\,1}P^0$ states of helium-like ions (Z=2–10). The results are expressed in Rydberg: 1Ry=13.6056925 eV.

States $^1P^o$	Z								
$_n(0,1)_N^+$	2	3	4	5	6	7	8	9	10
$_3(0,1)_2^+$	1.12451	2.72086	5.03943	8.08023	11.84325	16.32849	21.53595	27.46563	34.11754
$_4(0,1)_2^+$	1.08917	2.55098	4.63778	7.34959	10.68639	14.64820	19.23501	24.44681	30.28362
$_5(0,1)_2^+$	1.04305	2.41604	4.36904	6.90203	10.01502	13.70802	17.98101	22.83400	28.26700
$_6(0,1)_2^+$	1.02956	2.36464	4.25529	6.70148	9.70324	13.26055	17.37341	22.04183	27.26580
$_7(0,1)_2^+$	1.02096	2.33273	4.18531	6.57872	9.51293	12.98797	17.00382	21.56049	26.65797
$_8(0,1)_2^+$	1.01611	2.31348	4.14209	6.50195	9.39306	12.81542	16.76904	21.25390	26.27001
$_9(0,1)_2^+$	1.01299	2.30066	4.11303	6.45008	9.31183	12.69827	16.60940	21.04522	26.00573
$_{10}(0,1)_2^+$	1.01070	2.29138	4.09206	6.41275	9.25343	12.61412	16.49480	20.89549	25.81817