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Energy resonances for $^1P^o$, $^1D^e$, $^1F^o$, $^1G^e$, and $^1H^o$ autoionizing states of the helium isoelectronic series below the $n=2$–4 hydrogenic thresholds

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Abstract. General formalism of special form of Hylleraas correlated wave functions (SFHCWF) is demonstrated in this paper. The adequacy of the SFHCWF in the description as well as of the singlet than of the triplet excited states of two electron systems is also presented in this work. Application of SFHCWF to the calculations of doubly excited $nln'l'$ states $(n=2$–$4)$ in the helium-like ions is done, using the screening constant by unit nuclear charge method in the framework of a variational procedure. Comparison with various available theoretical and experimental literature values indicates a good agreement.

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Key words: energy resonances, helium isoelectronic series, special form of Hylleraas correlated wave functions, screening constant by unit nuclear charge, He-like ions

1 Introduction

The most suitable approached method used for the treatment of the ground state of two electron systems is the Ritz variational principal which has been first applied to the helium atom by Kellner [1] and with even great success by Hylleraas [2]. Since the early experiment of Madden and Codling [3] and others [4] and theoretical explanation of Cooper, Fano and Prats [5], doubly-excited states (DES) of the helium-like ions have been the intention of several studies. Besides, higher-energy Rydberg envelopes contain doubly-excited states which are generally labelled in the usual spectroscopic notation $(Nl,nl')^{2S+1}\ L^{\pi}$ with $n=N$, $N+1,\cdots$ [6]. In these notations, N and n denote respectively the principal quantum numbers of the inner and the outer electron, l and l' there respective orbital quantum numbers, S the total spin, L the total angular momentum and π the parity of the system.

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Investigations of DES in two electron systems are of interest in spectroscopic diagnostic in connexion with the understanding of collisional and radiational processes taking place in hot astrophysical and laboratory plasmas [7]. For autoionizing states in the helium isoelectronic series, many computational methods are employed. Among these methods are, the computing double sum method over the complete hydrogen spectrum [8], the complex-coordinate rotation [9–12], the density functional theory [24], the Feshbach-projection method [14], the screening constant by unit nuclear charge (SCUNC) method [15–17] (to name a few). Special type of trial wave functions combining Hylleraas and incomplete hydrogenic wave functions have also been used in the computations of energies for doubly excited states of two electron systems [18–21]. But in these studies, the special form of Hylleraas correlated wave functions (SFHCWF) used by Biaye and co-workers [18–21], has been constructed by an iterative procedure.

In this paper, we present the general mathematical formalism that leads to the construction of such special wave functions. The adequacy of the SFHCWF in the description as well as of the singlet than of the triplet excited states of two electron systems is also presented. Besides, using the SCUNC- method, we apply SFHCWF in the calculations of $2s2p\,^1P^o$, $3s3p\,^1P^o$, $4s4p\,^1P^o$, $3s3d\,^1D^e$, $4s4d\,^1D^e$, $4s4f\,^1F^o$, $4p4d\,^1F^o$, $4p4f\,^1G^e$ and $4d4f\,^1H^o$ DES in He-like ions up to $Z=10$.

The advantages of the SCUNC method are connected with the possibilities to investigate autoionizing states in two-electron systems using either a variational or a semi-empirical procedure. Comparison of the results obtained with various theoretical other results is made. Discussions between the two procedures (semi-empirical and variational) of the SCUNC method are also made. In Section 2, we present the theoretical procedure adopted in this work. In Section 3, we present and discuss the results obtained, compared to available theoretical and experimental literature values.

2 SfHCWF for doubly excited states of two electron systems

For the ground state of two electron systems, the Hylleraas wave function is in the form

$$\Phi_{jkm}(\vec{r_1},\vec{r_2}) = (r_1+r_2)^j (r_1-r_2)^k |\vec{r_1}-\vec{r_2}|^m \exp -\lambda(r_1+r_2). \tag{1}$$

In this expression, $\vec{r_1}$ and $\vec{r_2}$ denote the positions of the two electrons, r_1 and r_2 are used respectively for $|\vec{r_1}|$ and $|\vec{r_2}|$, j, k, m are Hylleraas parameters satisfying the double condition (j, k, $m \geq 0$) and $j+k+m \leq 3$, λ represents a coefficient given by: $\lambda = Z/\alpha r_0$, where Z, α and r_0 denote respectively the nuclear charge number, the variational parameter and the Bohr's radius. The set of the parameters (j, k, m) define the basis states and then give their dimension D. From the theoretical viewpoint, the Hylleraas variational method is based on the Hylleraas and Undheim theorem [22] according to which, a good approximation of the energy eigenvalue $E(\alpha)$ is obtained when the minima of the function ($\mathrm{d}E(\alpha)/\mathrm{d}\alpha$=0) converge with increasing values of the dimension D of the basis states and when the function exhibit a plateau. In the Hylleraas wave function, the angular part corresponding to the spherical