J. At. Mol. Sci.
doi: 10.4208/jams.022510.031010a

Vol. **1**, No. 2, pp. 103-117
May 2010

A modification of atomic orbital theory and its application to $(1snl)^1L^\pi$ and $(nl^2)^1L^\pi$ excited states of He-like ions

I. Sakho*

UFR Sciences and Technologies, Department of Physics, University of Ziguinchor, Ziguinchor, Senegal

Received 25 Feburary 2010; Accepted (in revised version) 10 March 2010;
Available online 19 April 2010

Abstract. A modification of the Slater's atomic orbital theory (AOT) is presented in this paper and applied to the calculation of energies for $(1sns)^1S^e$, $(1snp)^1P^o$, $(1snd)^1D^e$ and $(ns^2)^1S^e$, $(np^2)^1D^e$, $(nd^2)^1G^e$, $(nf^2)^1I^e$, $(ng^2)^1K^e$, $(nh^2)^1M^e$ excited states of He-like ions up to Z = 12. The inadequacy of Slater's AOT for excited states of the atomic systems is discussed. The results obtained in the present work are in good agreement with available experimental and theoretical results.

PACS: 31.15.bu, 31.15.vj

Key words: atomic orbital theory, screening constant, semi-empirical calculations, excited states, helium-like ions

1 Introduction

Since the early experiment of Madden and Codling [1] and others [2] and theoretical explanation of Cooper, Fano and Prats [3], doubly-excited states (DES) of helium-like ions have been the intention of several studies. Greatest attention has been concentrated on the study of symmetric DES (nl^2) where the electronic correlation effects may be predominant as shown by Fano [4]. Some of these symmetric DES in two-electron systems have been identified in the solar flare [5] and in the solar corona [6] and, revealed experimentally by the studies of double Rydberg resonances in negative ions of rare gases [7,8]. 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 [9]. In this notation, 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

*Corresponding author. *Email address:* aminafatima_sakho@yahoo.fr (I. Sakho)

spin, L the total angular momentum and π the parity of the system. The lowest-energy envelope (N = 1) contains the singly-excited states $(1s,nl)^{2S+1}L^{\pi}$ approaching the first ionization threshold which have been over the years, the intention of some computations [10–12].

As concern the methods applied in the treatment of the helium-like atoms' properties in excited states, several techniques of computation have been performed. Among these methods are the hyperspherical close-coupling method [11], the method of computing double sums over the complete hydrogen spectrum [12], the diagonalization approximation [13–16] the variational method using the Hylleraas-type wave function [17, 18], the time-dependent variation perturbation theory [19], the variational method using the Pekeris-type electronic wavefunctions [20], the density-functional theory [21], the complex rotation method [22]. In all these *ab initio* methods, energies for excited states of He-like ions can't be expressed in a simple analytical formula. However, most of the preceding methods require large basis-set calculations involving a fair amount of mathematics complexity. But, it is widely believed that there are distinct advantages to viewing problems of physics within the framework of simple analytical models. Such analytical procedures have been performed successfully in the case of the ground -state of helium -like ions by Bethe and Salpeter [22] who express an excellent semi-empirical expansion for the first ionization energy of two-electron systems whereas Slater [24] developed his atomic orbital theory in the framework of a general semi-empirical approach and expresses analytical the total energy of an electronic configuration given containing several electrons.

Recently, Sakho [25] presents screening constant by unit nuclear charge analytical method very suitable for ground-state [26] and doubly excited states [25,27,28] of the helium isoelectronic sequence. Besides, if single-exponent Slater function [29] and complex-exponent Slater-orbitals [30] are employed in the study of the properties of atoms and molecules, the AOT as presented by Slater [24] is not suitable for excited states of atomic systems.

As AOT of Slater [24] is a suitable analytical approach for the ground state of atoms and isoelctronic ions, it will be interesting to present a modification of the Slater's AOT for excited states of atoms -like ions. Such study is the intention of this paper considering the particularly case of helium -like systems. In Section 2 we present our modification of the atomic orbital theory of Slater [24] after discussing its inadequacy for excited states of atomic systems. In Section 3, the presentation and the discussion of our results in the case of $(1sns)^1S^e$, $(1snp)^1P^o$, $(1snd)^1D^e$ and $(ns^2)^1S^e$, $(np^2)^1D^e$, $(nd^2)^1G^e$, $(nf^2)^1I^e$, $(ng^2)^1K^e$, $(nh^2)^1M^e$ excited states of He-like ions up to Z = 12 are made. All our results are compared to available theoretical and experimental data.