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General formalism of the modified atomic orbital theory for the Rydberg series of atoms and ions: application to the photoionization of Ne^+

I. Sakho*

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

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Abstract. The general formalism of the Modified orbital atomic theory (MAOT) for the Rydberg series of atoms and ions is presented. Energy resonances of the $2s^22p^4(^1D_2)ns$, nd, $2s^22p^4(^1S_0)ns,nd$ and $2s^2p^5(^3P_2)np$ Rydberg series originating from the $2s^22p^5$ $^2P_{1/2}$ metastable and from the $2s^22p^5$ $^2P_{3/2}$ ground state of Ne^+ are tabulate applying the MAOT formalism. Analysis of the present results is achieved in the framework of the standard quantum defect expansion formula. Comparison is done with the existing experimental and theoretical data.

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Key words: Modified atomic orbital theory (MAOT); Electron correlation calculations for atoms and ions; Rydberg series

1 Introduction

Photoionization of ions is seen to be a fundamental process of importance in many high-temperature plasma environments such as those in stars and nebulae [1] and those in inertial-confinement fusion experiments [2]. Quantitative measurements of photoionization of ions provide precision data on ionic structure, and guidance to the development of theoretical models of multielectron interactions [3]. These measurements are performed mainly using synchrotron radiations such as ASTRID (Aarhus STorage RIng in Denmark) [4], SOLEIL (Source Optimisée de Lumière d'Energie Intermédiaire du LURE (Laboratoire pour l'Utilisation du Rayonnement Electromagntique) in France [5], ALS (Advanced Light Source) in USA [3] and Spring 8 in Japon [6]. The development of these synchrotron light sources has provide high accurate experimental data for benchmarking state-of-the-art theoretical methods of calculations. Among these methods are the

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

Hartree-Fock multi-configurationnal (MCDF) method [7, 8], the Quantum Defect Theory [9], the R-matrix approach [10] widely used for international collaborations such as the Opacity Project [11, 12] or the Iron Project [13], the Screening constant by unit nuclear charge (SCUNC) formalism [14, 15]. As far as various ions of great importance for plasma diagnostics are concerned, those of the neon element are one of the prominent candidates due to their frequent use in tokomaks as a diagnostic element for probing plasma [16]. In addition, neon is known to be the sixth most abundant element in the universe and then is of great interest in astrophysics in connection with the role of neon ions in the interpretation of astronomical data from stellar objects such as gaseous nebulas. At ultraviolet wavelengths in the range 300-90 Å, corresponding to a photon energy range of 41 - 138 eV, radiation can photoionize the ground states of several ionization stages of neon such as Ne^+, Ne^{2+}, Ne^{3+}, and Ne^{4+}, leaving the residual ion in one of several excited states [3]. These ions and those of carbon (C^{2+}, C^{3+}, C^{4+}), of nitrogen (N^{2+}, N^{3+}, N^{4+}) and of oxygen (O^{2+}, O^{3+}, O^{4+}) are known to contribute to the opacity in the atmospheres of the central stars of planetary nebulas [17, 18]. Using the Advanced Light Source (ALS) devices, Covington *et al.*, [3] presented both high-resolution absolute measurements and theoretical calculations of Ne^+ at photon energies ranging from the photoionization threshold to 70 eV. These experiments were focused on the $2s^22p^4(^1D_2)ns,nd$, $2s^22p^4(^1S_0)ns,nd$ and $2s^2p^5(^3P_2)np$ Rydberg series originating from both $2s^22p^5\ ^2P_{1/2}$ metastable and $2s^22p^5\ ^2P_{3/2}$ ground state of Ne^+. Very recently, Faye *et al.*, [15] used the Screening constant by unit nuclear charge (SCUNC) method to report high lying energy positions of the preceding series. In general, the availability of high-resolution measurements data on ionic species provides great opportunities to verify the accuracy of theoretical predictions or the limitations of a given quantum mechanics model. For this purpose, the General formalism of the Modified orbital atomic theory (MAOT) [19-22] for the Rydberg series of atoms and ions is presented and applied to the photoionization of Ne^+ considering the same above Rydberg states. Section 2 presents the theoretical procedure adopted in this work. In Section 3, we present and discuss the results obtained, compared to available literature data.

2 Theory

2.1 Brief description of the MAOT formalism

In the framework of the Modified Atomic Orbital Theory (MAOT), total energy of a $(\nu\ell)$-given orbital is expressed in the form [19, 20]

$$E(\nu\ell) = -\frac{[Z-\sigma(\ell)]^2}{\nu^2}. \tag{1}$$

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

$$E = -\sum_{i=1}^{M}\frac{[Z-\sigma_i(\ell)]^2}{\nu_i^2}.$$